



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 02:44 PM UTC

PDB ID : 2LVZ / pdb_00002lvz
BMRB ID : 18596
Title : Solution structure of a Eosinophil Cationic Protein-trisaccharide heparin mimetic complex
Authors : Garcia Mayoral, M.; Canales, A.; Diaz, D.; Lopez Prados, J.; Moussaoui, M.; de Paz, J.; Angulo, J.; Nieto, P.; Jimenez Barbero, J.; Boix, E.; Bruix, M.
Deposited on : 2012-07-17

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

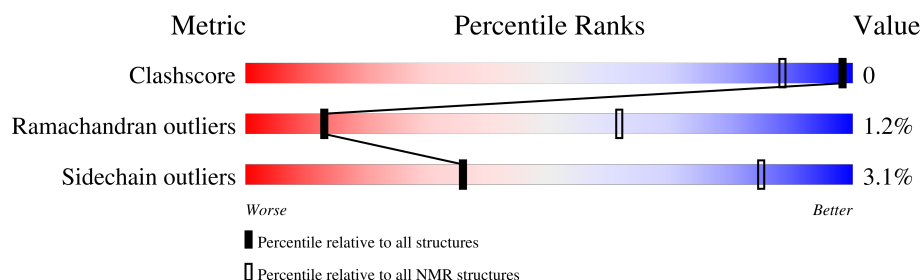
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	133	
2	B	3	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:133 (132)	0.75	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	11, 12, 13, 14, 17, 18
2	5, 6, 8
3	4, 15, 16
4	1, 2
Single-model clusters	3; 7; 9; 10; 19; 20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2259 atoms, of which 1107 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Eosinophil cationic protein.

Mol	Chain	Residues	Atoms						Trace
1	A	133	Total	C	H	N	O	S	0
			2169	677	1075	224	184	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ARG	THR	conflict	UNP P12724

- Molecule 2 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside.

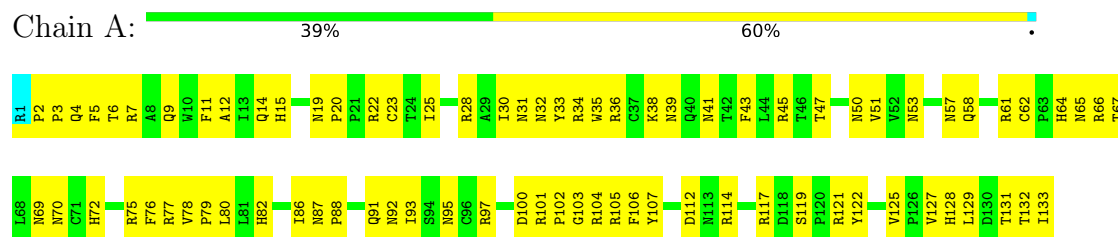
Mol	Chain	Residues	Atoms						Trace
2	B	3	Total	C	H	N	O	S	0
			90	21	32	2	30	5	

4 Residue-property plots [i](#)

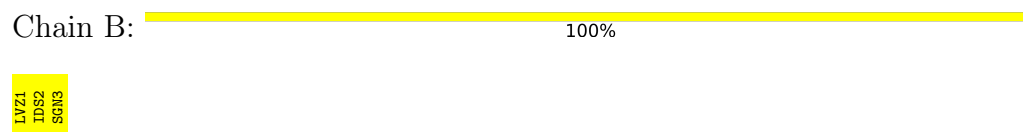
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Eosinophil cationic protein



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

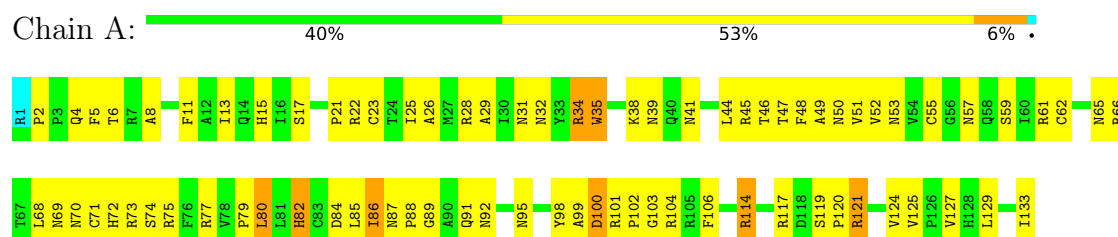


4.2 Scores per residue for each member of the ensemble

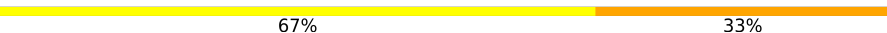
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Eosinophil cationic protein



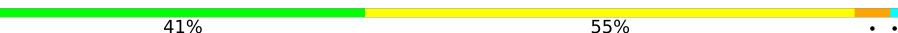
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain B:  67% 33%

LVZ1
IDS2
SGN3

4.2.2 Score per residue for model 2

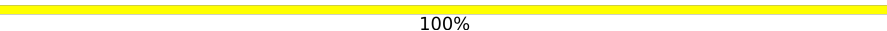
- Molecule 1: Eosinophil cationic protein

Chain A:  41% 55% ..

R1 P2 P3 P4 Q4 F5 T6 R7 W10 F11 A12 I13 Q14 H15 I16 S17 L18 N19 P20 P21 R22 A26 M27 R28 A29 I30 N31 N32 Y33 R34 Y35 R36 K37 K38 N39 Q40 N41 T46 V51 V54 C55 G56 N57 I60 R61 C62 P63 H64 N65 R66 T67 L68 N69 C71

H72 R73 S74 R75 F76 R77 L80 L81 H82 C83 D84 L85 L86 N87 P88 G89 A90 Q91 Q92 I93 C96 R97 Y98 R101 R104 R105 F106 Y107 D112 N113 R114 D115 R116 R117 D118 S119 P120 P121 Y122 P123 V124 V125 V126 P127 H128 L129 D130 T131 T132 I133

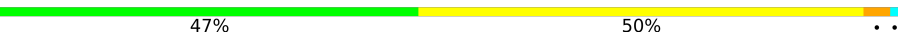
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain B:  100%

LVZ1
IDS2
SGN3

4.2.3 Score per residue for model 3

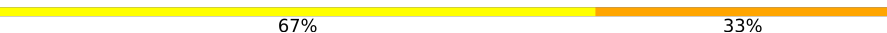
- Molecule 1: Eosinophil cationic protein

Chain A:  47% 50% ..

R1 P2 P3 Q4 F5 T6 R7 W10 F11 A12 H15 L18 N19 P20 R21 R22 C23 T24 I25 A26 M27 R28 A29 I30 N31 N32 Y33 R34 K38 N39 Q40 N41 R45 N50 N53 V54 C55 S59 I60 R61 C62 P63 H64 N65 R66 T67 H72 R73 V78 P79

L80 L81 H82 C83 D84 L85 L86 N87 P88 G89 A90 Q91 N92 N95 Y98 A99 D100 P101 P102 G103 R104 R105 F106 Y107 D115 P116 R117 D118 S119 P120 R121 Y122 V125 H128 L129 D130 T131 T132 I133

- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

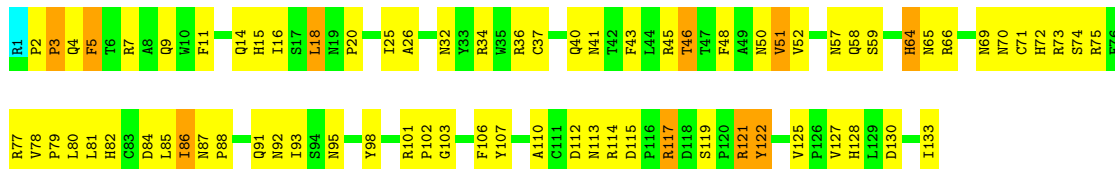
Chain B:  67% 33%

LVZ1
IDS2
SGN3

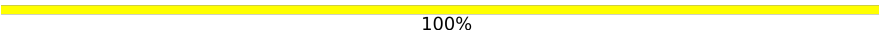
4.2.4 Score per residue for model 4

- Molecule 1: Eosinophil cationic protein

Chain A:  43% 49% 8%



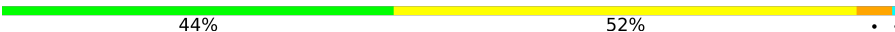
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

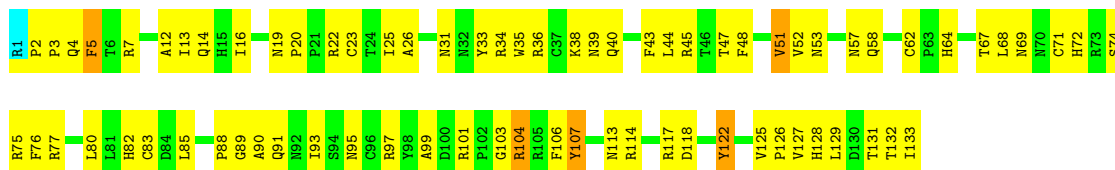
Chain B:  100%

LVZ1
IDS2
SGN3

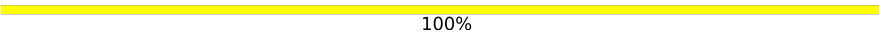
4.2.5 Score per residue for model 5

- Molecule 1: Eosinophil cationic protein

Chain A:  44% 52%



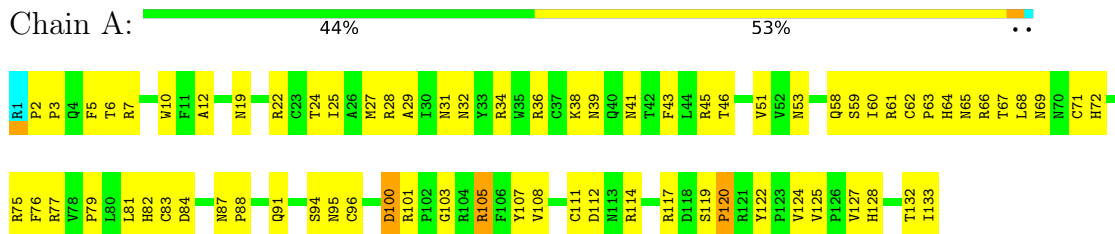
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain B:  100%

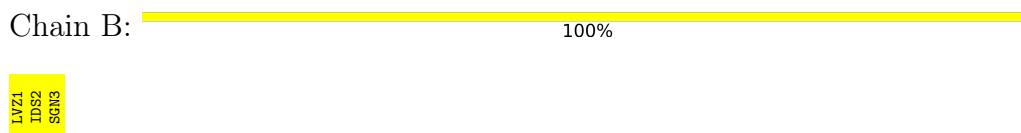
LVZ1
IDS2
SGN3

4.2.6 Score per residue for model 6

- Molecule 1: Eosinophil cationic protein

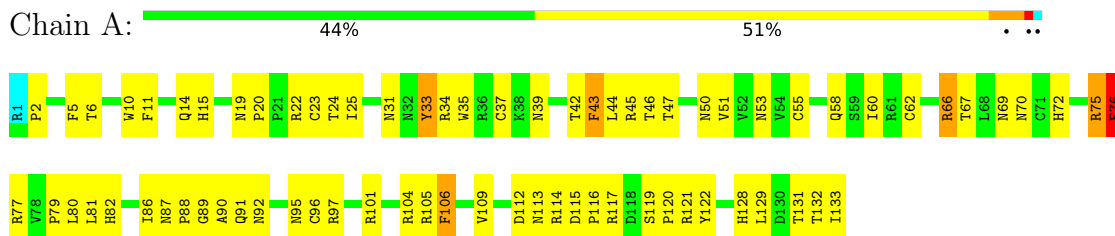


- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

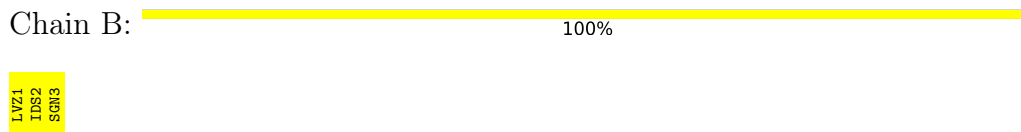


4.2.7 Score per residue for model 7

- Molecule 1: Eosinophil cationic protein



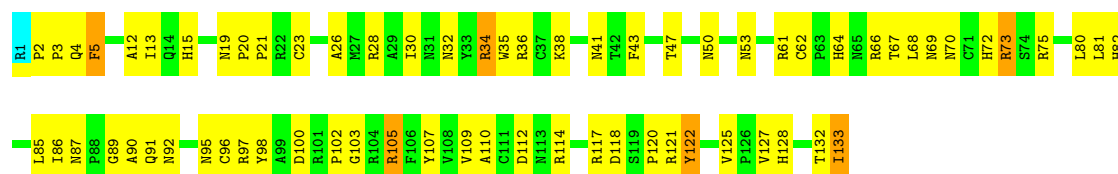
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside



4.2.8 Score per residue for model 8

- Molecule 1: Eosinophil cationic protein





- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

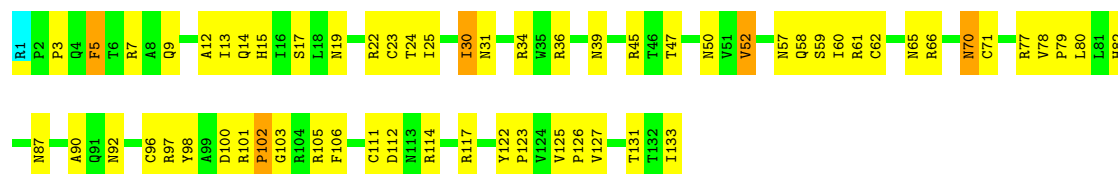
Chain B: 100%

LVZ1
IDS2
SGN3

4.2.9 Score per residue for model 9

- Molecule 1: Eosinophil cationic protein

Chain A: 53% 42% ..



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

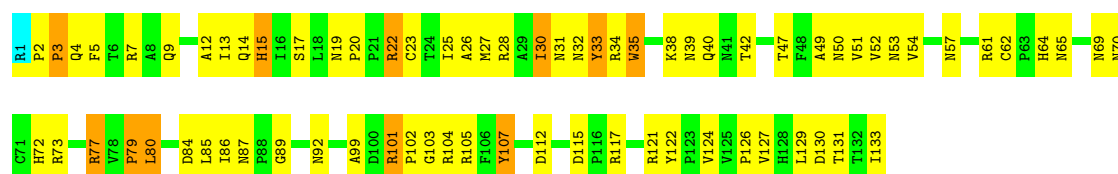
Chain B: 100%

LVZ1
IDS2
SGN3

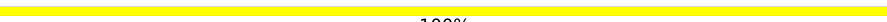
4.2.10 Score per residue for model 10

- Molecule 1: Eosinophil cationic protein

Chain A: 44% 47% 8% ..



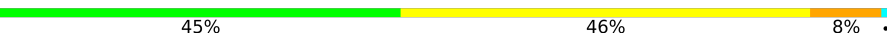
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

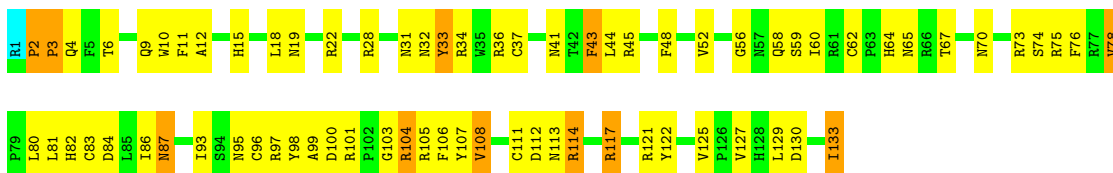
Chain B:  100%

LVZ1
IDS2
SGN3

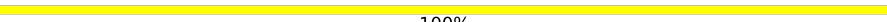
4.2.11 Score per residue for model 11

- Molecule 1: Eosinophil cationic protein

Chain A:  45% 46% 8%



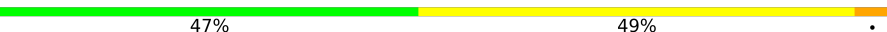
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

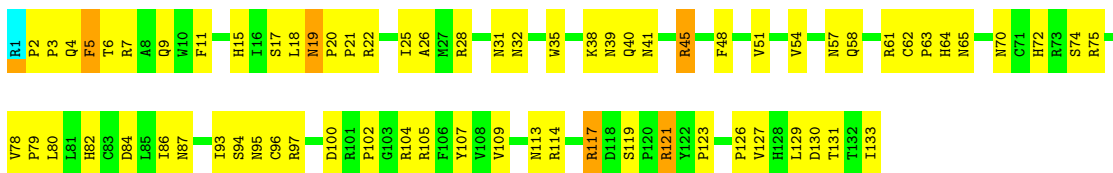
Chain B:  100%

LVZ1
IDS2
SGN3

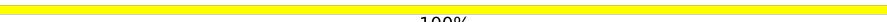
4.2.12 Score per residue for model 12

- Molecule 1: Eosinophil cationic protein

Chain A:  47% 49%



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

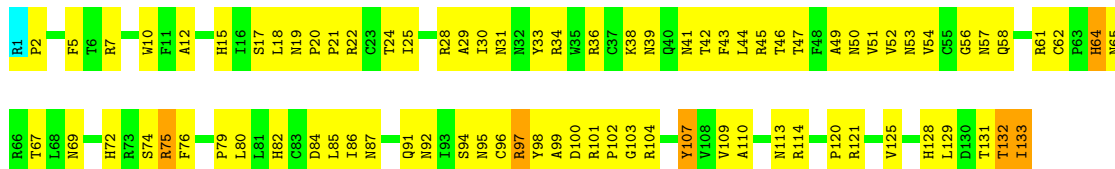
Chain B:  100%

LVZ1
IDS2
SGN3

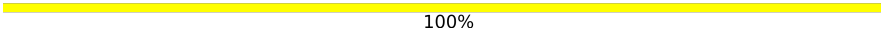
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Eosinophil cationic protein

Chain A:  38% 57% 5%



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

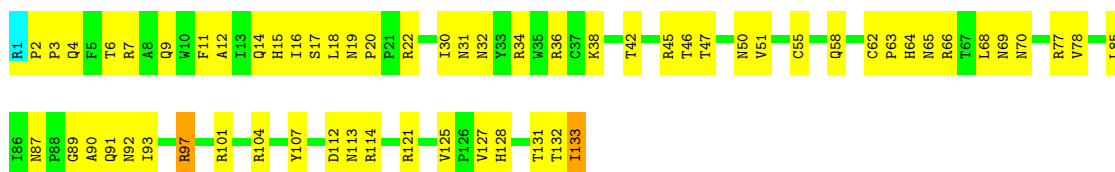
Chain B:  100%

LVZ1
IDS2
SGN3

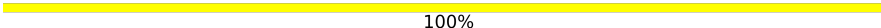
4.2.14 Score per residue for model 14

- Molecule 1: Eosinophil cationic protein

Chain A:  53% 44% ..



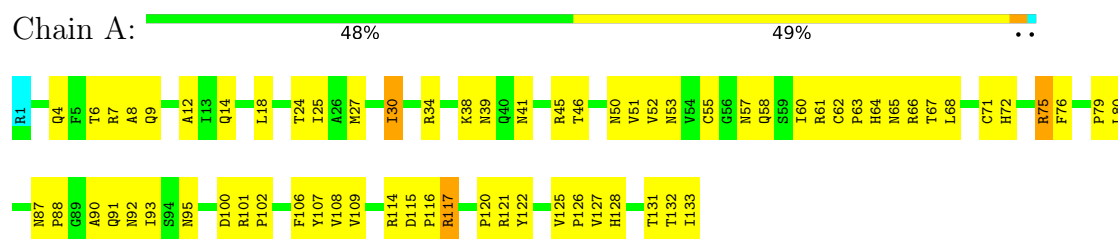
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain B:  100%

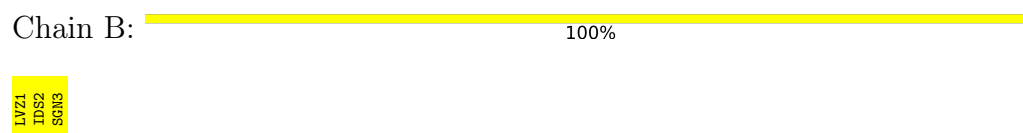
LVZ1
IDS2
SGN3

4.2.15 Score per residue for model 15

- Molecule 1: Eosinophil cationic protein

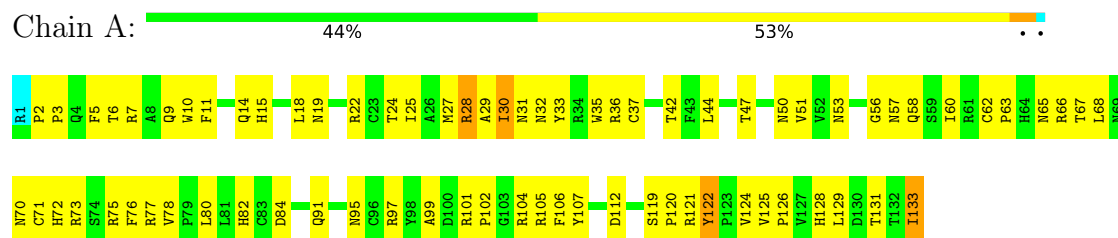


- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

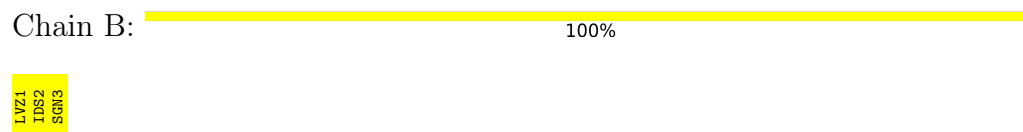


4.2.16 Score per residue for model 16

- Molecule 1: Eosinophil cationic protein



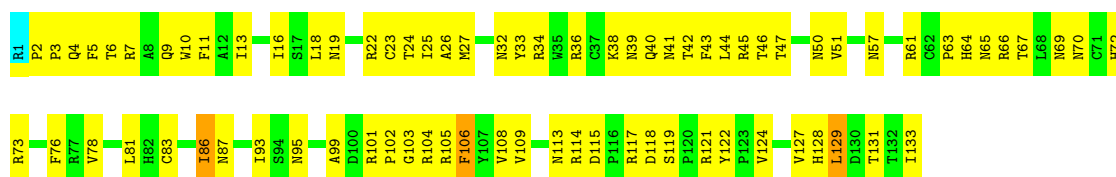
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside



4.2.17 Score per residue for model 17

- Molecule 1: Eosinophil cationic protein





- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

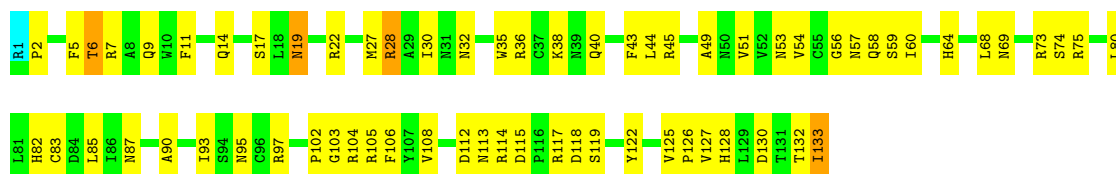
Chain B: 100%

LVZ1
IDS2
SGN3

4.2.18 Score per residue for model 18

- Molecule 1: Eosinophil cationic protein

Chain A: 50% 47% ..



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

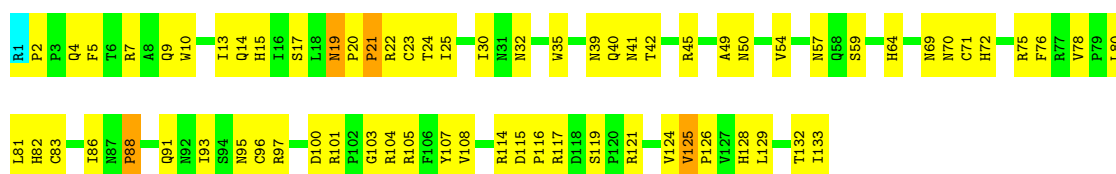
Chain B: 100%

LVZ1
IDS2
SGN3

4.2.19 Score per residue for model 19

- Molecule 1: Eosinophil cationic protein

Chain A: 47% 49% ..



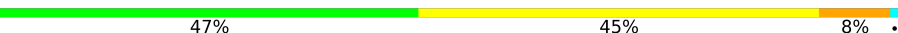
- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

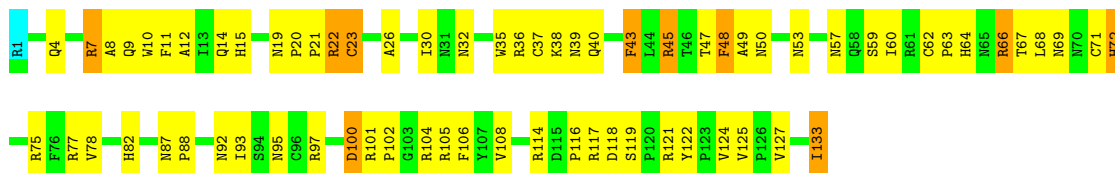
Chain B:  100%

LVZ1
IDS2
SGN3

4.2.20 Score per residue for model 20

- Molecule 1: Eosinophil cationic protein

Chain A:  47% 45% 8%



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain B:  100%

LVZ1
IDS2
SGN3

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Amber	structure solution	
CYANA	structure solution	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1481
Number of shifts mapped to atoms	1481
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LVZ, IDS, SGN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.12±0.05	31±3/1113 (2.8± 0.3%)	2.46±0.06	73±10/1515 (4.8± 0.7%)
All	All	2.12	613/22260 (2.8%)	2.46	1465/30300 (4.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.8±2.1
All	All	0	115

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	62	CYS	CA-C	11.15	1.63	1.52	14	4
1	A	119	SER	CA-CB	11.02	1.60	1.52	18	3
1	A	78	VAL	CA-CB	10.07	1.66	1.55	3	1
1	A	104	ARG	CA-C	9.91	1.64	1.52	11	1
1	A	80	LEU	CA-C	9.85	1.64	1.52	2	3
1	A	119	SER	CA-C	9.65	1.59	1.53	4	2
1	A	98	TYR	CA-C	9.05	1.63	1.52	11	2
1	A	6	THR	N-CA	8.86	1.57	1.45	17	3
1	A	38	LYS	N-CA	8.74	1.56	1.46	15	2
1	A	19	ASN	CA-CB	8.68	1.64	1.53	18	1
1	A	90	ALA	CA-C	8.61	1.63	1.52	14	3
1	A	82	HIS	ND1-CE1	8.41	1.41	1.32	9	9
1	A	25	ILE	C-O	-8.35	1.14	1.23	7	2
1	A	120	PRO	N-CA	8.34	1.57	1.47	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	ASN	CA-C	8.32	1.59	1.52	9	3
1	A	82	HIS	CE1-NE2	8.30	1.40	1.32	3	1
1	A	89	GLY	CA-C	8.25	1.62	1.51	8	1
1	A	19	ASN	CA-C	8.24	1.63	1.52	14	3
1	A	125	VAL	CA-C	8.22	1.61	1.52	3	6
1	A	126	PRO	N-CA	-8.21	1.37	1.47	19	2
1	A	30	ILE	CA-C	8.16	1.61	1.52	18	1
1	A	33	TYR	CA-C	8.15	1.63	1.52	11	1
1	A	119	SER	C-O	8.12	1.27	1.23	16	3
1	A	2	PRO	CA-C	8.08	1.59	1.52	11	5
1	A	29	ALA	CA-C	8.06	1.63	1.52	6	2
1	A	4	GLN	CA-C	8.04	1.62	1.53	5	4
1	A	109	VAL	N-CA	8.02	1.54	1.46	12	1
1	A	34	ARG	N-CA	8.00	1.56	1.45	6	3
1	A	58	GLN	CA-C	7.98	1.62	1.52	12	2
1	A	21	PRO	CA-C	7.91	1.61	1.52	12	1
1	A	44	LEU	CA-C	7.90	1.63	1.52	1	2
1	A	63	PRO	N-CD	-7.90	1.36	1.47	12	2
1	A	103	GLY	CA-C	7.89	1.61	1.51	6	6
1	A	96	CYS	CA-C	7.88	1.62	1.52	8	2
1	A	41	ASN	N-CA	7.87	1.55	1.45	4	2
1	A	62	CYS	N-CA	-7.86	1.40	1.46	5	4
1	A	128	HIS	CD2-NE2	7.75	1.46	1.37	14	2
1	A	94	SER	N-CA	7.73	1.56	1.46	6	2
1	A	97	ARG	CD-NE	7.73	1.57	1.46	11	2
1	A	39	ASN	C-N	7.69	1.43	1.33	13	1
1	A	20	PRO	CA-C	7.68	1.59	1.52	2	7
1	A	25	ILE	CA-CB	-7.65	1.47	1.55	10	1
1	A	59	SER	CA-C	7.64	1.62	1.52	3	2
1	A	32	ASN	CA-C	7.64	1.62	1.53	12	4
1	A	73	ARG	CA-C	7.59	1.61	1.52	4	1
1	A	75	ARG	NE-CZ	-7.58	1.24	1.33	19	1
1	A	43	PHE	CA-C	7.49	1.61	1.52	17	2
1	A	71	CYS	CA-C	7.49	1.62	1.52	9	2
1	A	103	GLY	N-CA	7.43	1.51	1.45	8	3
1	A	84	ASP	CA-C	7.39	1.60	1.52	1	2
1	A	130	ASP	CA-C	7.39	1.59	1.52	18	2
1	A	22	ARG	N-CA	7.39	1.55	1.45	16	3
1	A	97	ARG	CZ-NH2	-7.37	1.23	1.33	7	3
1	A	93	ILE	CA-C	7.33	1.62	1.52	18	3
1	A	40	GLN	CA-C	7.31	1.61	1.52	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	13	ILE	CA-C	7.26	1.61	1.52	2	2
1	A	76	PHE	CA-C	7.25	1.61	1.52	19	3
1	A	15	HIS	CA-C	7.23	1.60	1.52	19	2
1	A	47	THR	CA-C	7.20	1.61	1.52	9	2
1	A	72	HIS	ND1-CE1	7.20	1.39	1.32	10	3
1	A	68	LEU	CA-C	7.16	1.62	1.52	1	2
1	A	15	HIS	CE1-NE2	7.16	1.39	1.32	3	4
1	A	5	PHE	CA-C	7.14	1.61	1.52	19	4
1	A	70	ASN	CA-C	7.13	1.61	1.52	16	4
1	A	108	VAL	N-CA	7.13	1.55	1.46	6	3
1	A	54	VAL	CA-C	7.13	1.62	1.52	13	1
1	A	127	VAL	N-CA	7.12	1.52	1.46	6	5
1	A	101	ARG	CA-C	7.12	1.61	1.52	1	4
1	A	37	CYS	N-CA	7.09	1.55	1.46	4	1
1	A	115	ASP	CA-C	7.08	1.60	1.53	15	2
1	A	73	ARG	C-N	-7.06	1.24	1.33	10	1
1	A	86	ILE	N-CA	7.06	1.55	1.46	13	2
1	A	90	ALA	N-CA	7.04	1.54	1.46	15	1
1	A	127	VAL	CA-C	7.03	1.61	1.52	14	4
1	A	53	ASN	CA-C	7.03	1.62	1.52	15	1
1	A	61	ARG	CD-NE	7.01	1.56	1.46	12	1
1	A	48	PHE	CA-CB	7.01	1.64	1.53	12	1
1	A	122	TYR	CA-C	6.92	1.58	1.52	5	2
1	A	52	VAL	N-CA	6.92	1.54	1.46	9	1
1	A	3	PRO	N-CA	-6.92	1.38	1.47	6	1
1	A	44	LEU	CA-CB	6.89	1.64	1.53	7	1
1	A	82	HIS	CG-ND1	-6.89	1.30	1.38	12	2
1	A	57	ASN	N-CA	6.87	1.53	1.45	12	1
1	A	126	PRO	CA-C	-6.84	1.43	1.52	15	1
1	A	104	ARG	N-CA	6.84	1.54	1.46	20	1
1	A	101	ARG	N-CA	6.80	1.54	1.46	1	3
1	A	33	TYR	N-CA	6.77	1.55	1.46	7	3
1	A	61	ARG	CZ-NH1	-6.77	1.23	1.32	6	3
1	A	73	ARG	N-CA	6.77	1.54	1.45	8	2
1	A	65	ASN	N-CA	6.73	1.52	1.46	9	1
1	A	28	ARG	NE-CZ	-6.73	1.25	1.33	3	2
1	A	84	ASP	N-CA	6.71	1.54	1.46	11	1
1	A	7	ARG	CZ-NH2	-6.71	1.24	1.33	13	3
1	A	64	HIS	CE1-NE2	6.70	1.39	1.32	11	3
1	A	30	ILE	CA-CB	6.69	1.63	1.54	10	2
1	A	81	LEU	CA-C	6.69	1.60	1.52	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	102	PRO	C-N	6.68	1.39	1.33	3	1
1	A	72	HIS	CE1-NE2	6.67	1.39	1.32	15	4
1	A	85	LEU	CA-C	6.67	1.60	1.53	3	2
1	A	108	VAL	C-O	6.67	1.30	1.24	15	1
1	A	132	THR	N-CA	6.66	1.54	1.46	19	2
1	A	64	HIS	C-O	-6.63	1.18	1.24	3	1
1	A	124	VAL	N-CA	6.58	1.53	1.46	2	2
1	A	36	ARG	CA-C	6.57	1.60	1.52	18	3
1	A	67	THR	CA-C	6.55	1.61	1.52	3	2
1	A	95	ASN	CA-C	6.54	1.60	1.52	15	2
1	A	112	ASP	CA-CB	6.53	1.64	1.53	7	1
1	A	61	ARG	C-N	6.53	1.41	1.33	8	2
1	A	125	VAL	N-CA	6.50	1.54	1.46	3	3
1	A	128	HIS	ND1-CE1	6.49	1.39	1.32	7	2
1	A	22	ARG	CZ-NH1	-6.48	1.23	1.32	14	1
1	A	106	PHE	N-CA	6.48	1.54	1.45	16	3
1	A	9	GLN	CA-C	-6.46	1.44	1.52	11	1
1	A	82	HIS	CA-CB	6.46	1.62	1.53	6	1
1	A	62	CYS	CA-CB	6.44	1.61	1.53	6	2
1	A	128	HIS	CG-ND1	6.44	1.45	1.38	7	2
1	A	64	HIS	CD2-NE2	-6.43	1.30	1.37	20	1
1	A	79	PRO	CA-C	6.41	1.60	1.52	13	2
1	A	88	PRO	N-CA	6.40	1.55	1.47	6	2
1	A	62	CYS	C-N	6.40	1.41	1.34	6	1
1	A	87	ASN	N-CA	6.39	1.53	1.46	15	1
1	A	24	THR	N-CA	6.38	1.54	1.46	7	2
1	A	8	ALA	CA-C	6.37	1.61	1.52	20	2
1	A	17	SER	N-CA	6.34	1.55	1.47	1	2
1	A	7	ARG	N-CA	6.34	1.53	1.46	18	2
1	A	96	CYS	C-O	6.33	1.31	1.23	6	1
1	A	81	LEU	CA-CB	6.33	1.62	1.53	7	2
1	A	60	ILE	CA-C	6.33	1.60	1.53	3	1
1	A	69	ASN	CA-C	6.33	1.61	1.53	14	2
1	A	114	ARG	CZ-NH2	-6.30	1.25	1.33	5	1
1	A	79	PRO	CA-CB	6.30	1.62	1.53	10	1
1	A	125	VAL	C-N	6.29	1.41	1.33	1	2
1	A	15	HIS	ND1-CE1	6.29	1.38	1.32	11	2
1	A	110	ALA	CA-C	6.28	1.60	1.52	13	2
1	A	132	THR	CA-C	6.28	1.60	1.52	8	2
1	A	122	TYR	N-CA	6.27	1.53	1.45	20	2
1	A	32	ASN	N-CA	6.24	1.53	1.46	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	117	ARG	CZ-NH2	-6.24	1.25	1.33	8	4
1	A	44	LEU	N-CA	6.23	1.53	1.46	17	2
1	A	91	GLN	N-CA	6.22	1.53	1.46	16	3
1	A	71	CYS	N-CA	6.22	1.53	1.45	19	2
1	A	75	ARG	CZ-NH1	-6.19	1.24	1.32	12	2
1	A	3	PRO	CA-CB	-6.19	1.43	1.53	5	1
1	A	56	GLY	CA-C	6.19	1.59	1.51	18	2
1	A	51	VAL	CA-C	6.19	1.61	1.52	6	2
1	A	2	PRO	CA-CB	-6.17	1.45	1.54	10	2
1	A	45	ARG	CA-CB	6.17	1.60	1.52	7	2
1	A	60	ILE	N-CA	6.15	1.54	1.46	6	2
1	A	105	ARG	N-CA	6.14	1.53	1.46	8	2
1	A	49	ALA	N-CA	6.14	1.54	1.46	10	2
1	A	119	SER	N-CA	6.13	1.51	1.46	4	3
1	A	71	CYS	CA-CB	6.13	1.63	1.53	15	1
1	A	69	ASN	N-CA	6.13	1.54	1.46	8	2
1	A	51	VAL	N-CA	6.12	1.54	1.46	10	1
1	A	72	HIS	CA-C	-6.12	1.45	1.52	20	3
1	A	131	THR	CA-C	6.11	1.60	1.52	10	2
1	A	63	PRO	C-O	-6.10	1.16	1.24	2	1
1	A	65	ASN	CA-C	6.10	1.60	1.52	6	2
1	A	9	GLN	C-N	6.09	1.42	1.34	11	1
1	A	50	ASN	CA-C	6.09	1.60	1.52	19	2
1	A	101	ARG	CA-CB	-6.09	1.46	1.53	5	1
1	A	114	ARG	N-CA	6.09	1.53	1.46	18	1
1	A	118	ASP	N-CA	6.07	1.52	1.45	17	2
1	A	7	ARG	CA-C	6.06	1.60	1.52	2	1
1	A	77	ARG	NE-CZ	6.05	1.39	1.33	7	1
1	A	116	PRO	N-CD	-6.05	1.39	1.47	3	1
1	A	82	HIS	CA-C	6.03	1.59	1.52	20	1
1	A	121	ARG	CZ-NH2	-6.01	1.25	1.33	2	3
1	A	53	ASN	C-N	5.99	1.41	1.33	10	2
1	A	74	SER	N-CA	5.99	1.53	1.46	12	2
1	A	12	ALA	CA-C	5.99	1.60	1.52	2	2
1	A	85	LEU	CA-CB	5.99	1.60	1.52	10	1
1	A	67	THR	CB-OG1	-5.98	1.34	1.43	17	4
1	A	130	ASP	C-N	5.96	1.41	1.33	12	1
1	A	59	SER	N-CA	5.95	1.53	1.46	1	2
1	A	23	CYS	CA-C	5.94	1.60	1.52	17	1
1	A	34	ARG	CZ-NH2	-5.93	1.25	1.33	8	1
1	A	101	ARG	NE-CZ	-5.91	1.26	1.33	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	128	HIS	CB-CG	-5.91	1.41	1.50	8	1
1	A	92	ASN	CA-C	5.91	1.60	1.52	13	3
1	A	117	ARG	CD-NE	5.90	1.54	1.46	12	1
1	A	78	VAL	C-O	-5.89	1.20	1.24	17	2
1	A	97	ARG	N-CA	5.88	1.53	1.45	8	5
1	A	85	LEU	C-O	5.87	1.30	1.23	4	1
1	A	18	LEU	CA-CB	5.87	1.62	1.53	16	2
1	A	18	LEU	N-CA	5.87	1.53	1.46	15	1
1	A	6	THR	CA-CB	5.86	1.61	1.53	15	1
1	A	39	ASN	CA-CB	5.86	1.62	1.53	12	1
1	A	10	TRP	NE1-CE2	5.85	1.43	1.37	2	2
1	A	78	VAL	CA-C	-5.85	1.47	1.52	19	3
1	A	66	ARG	CZ-NH2	-5.84	1.25	1.33	3	2
1	A	90	ALA	CA-CB	5.84	1.62	1.53	9	1
1	A	103	GLY	C-N	5.83	1.40	1.33	10	1
1	A	26	ALA	CA-C	5.83	1.60	1.52	10	1
1	A	16	ILE	N-CA	5.83	1.54	1.46	2	1
1	A	12	ALA	N-CA	-5.82	1.39	1.46	8	1
1	A	34	ARG	NE-CZ	-5.81	1.26	1.33	17	1
1	A	34	ARG	CD-NE	5.81	1.54	1.46	6	1
1	A	124	VAL	C-N	5.80	1.40	1.33	20	1
1	A	128	HIS	CA-C	5.80	1.59	1.52	16	2
1	A	67	THR	N-CA	5.79	1.53	1.46	16	2
1	A	21	PRO	CA-CB	5.78	1.61	1.53	13	1
1	A	64	HIS	ND1-CE1	5.78	1.38	1.32	14	1
1	A	110	ALA	N-CA	5.78	1.52	1.45	4	1
1	A	75	ARG	N-CA	5.78	1.53	1.46	4	2
1	A	16	ILE	CB-CG1	5.77	1.65	1.53	17	1
1	A	46	THR	CB-OG1	-5.77	1.34	1.43	14	1
1	A	37	CYS	CA-C	5.77	1.60	1.52	2	1
1	A	118	ASP	CA-C	5.77	1.59	1.52	5	1
1	A	58	GLN	N-CA	5.76	1.53	1.46	16	2
1	A	114	ARG	CA-C	5.76	1.60	1.53	2	3
1	A	95	ASN	C-N	5.76	1.41	1.33	3	1
1	A	102	PRO	CA-CB	5.75	1.61	1.53	17	2
1	A	77	ARG	CZ-NH2	-5.74	1.25	1.33	5	1
1	A	117	ARG	N-CA	5.73	1.53	1.46	9	2
1	A	75	ARG	CZ-NH2	-5.73	1.26	1.33	4	1
1	A	105	ARG	CA-C	5.72	1.59	1.52	2	1
1	A	64	HIS	CA-C	5.72	1.60	1.52	20	2
1	A	91	GLN	CA-C	5.72	1.59	1.52	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	116	PRO	N-CA	5.72	1.54	1.47	20	3
1	A	46	THR	C-O	-5.71	1.17	1.24	2	1
1	A	128	HIS	CE1-NE2	5.71	1.38	1.32	5	4
1	A	129	LEU	C-N	5.71	1.41	1.33	17	1
1	A	39	ASN	N-CA	-5.70	1.39	1.46	12	1
1	A	85	LEU	C-N	5.70	1.40	1.34	1	1
1	A	126	PRO	C-N	5.69	1.38	1.33	15	1
1	A	66	ARG	CD-NE	5.68	1.54	1.46	14	1
1	A	66	ARG	CA-C	5.67	1.60	1.52	8	1
1	A	31	ASN	N-CA	5.66	1.53	1.46	13	1
1	A	72	HIS	CG-CD2	5.66	1.42	1.35	3	1
1	A	5	PHE	C-N	5.65	1.41	1.33	9	1
1	A	22	ARG	CZ-NH2	-5.65	1.26	1.33	9	2
1	A	128	HIS	CG-CD2	5.65	1.42	1.35	6	1
1	A	117	ARG	C-N	5.64	1.41	1.33	15	1
1	A	35	TRP	C-O	5.63	1.31	1.24	8	1
1	A	126	PRO	N-CD	-5.63	1.39	1.47	18	1
1	A	104	ARG	CZ-NH2	-5.63	1.26	1.33	18	4
1	A	27	MET	N-CA	5.62	1.53	1.46	10	1
1	A	41	ASN	CA-C	5.62	1.59	1.52	11	4
1	A	36	ARG	CZ-NH2	-5.61	1.26	1.33	6	3
1	A	77	ARG	C-N	5.61	1.38	1.33	20	1
1	A	101	ARG	CZ-NH2	-5.61	1.26	1.33	20	2
1	A	127	VAL	C-N	5.59	1.40	1.33	11	1
1	A	45	ARG	NE-CZ	-5.59	1.26	1.33	1	1
1	A	57	ASN	CA-C	5.59	1.61	1.53	2	3
1	A	83	CYS	CA-C	5.59	1.59	1.52	11	3
1	A	94	SER	C-N	-5.59	1.25	1.33	13	1
1	A	56	GLY	C-O	-5.58	1.17	1.23	13	1
1	A	15	HIS	CA-CB	5.56	1.62	1.54	9	1
1	A	26	ALA	C-N	5.55	1.41	1.33	20	1
1	A	46	THR	CA-CB	5.55	1.61	1.53	15	1
1	A	25	ILE	CA-C	5.54	1.60	1.52	3	2
1	A	76	PHE	N-CA	5.54	1.52	1.45	19	1
1	A	33	TYR	C-O	-5.53	1.17	1.24	5	1
1	A	36	ARG	N-CA	5.52	1.53	1.46	11	1
1	A	17	SER	CA-C	5.52	1.58	1.52	14	2
1	A	33	TYR	C-N	5.51	1.41	1.33	16	1
1	A	54	VAL	N-CA	5.50	1.53	1.46	10	2
1	A	78	VAL	N-CA	5.50	1.51	1.46	19	1
1	A	19	ASN	C-N	5.49	1.40	1.33	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	64	HIS	CG-CD2	5.49	1.41	1.35	8	1
1	A	10	TRP	CA-C	5.48	1.60	1.52	17	2
1	A	28	ARG	CZ-NH1	-5.48	1.25	1.32	16	2
1	A	94	SER	CA-CB	5.47	1.62	1.53	12	1
1	A	51	VAL	C-O	-5.47	1.17	1.24	16	1
1	A	23	CYS	N-CA	5.47	1.53	1.46	7	1
1	A	112	ASP	CA-C	5.46	1.59	1.52	18	2
1	A	34	ARG	CA-C	5.46	1.59	1.52	7	1
1	A	109	VAL	C-O	-5.45	1.17	1.24	17	1
1	A	45	ARG	CA-C	5.44	1.59	1.53	19	2
1	A	105	ARG	CZ-NH2	-5.44	1.26	1.33	2	2
1	A	105	ARG	NE-CZ	-5.44	1.27	1.33	10	1
1	A	77	ARG	CD-NE	5.44	1.53	1.46	6	1
1	A	6	THR	C-N	5.42	1.40	1.33	14	2
1	A	12	ALA	C-N	5.42	1.40	1.34	3	1
1	A	14	GLN	CA-C	5.41	1.60	1.52	5	2
1	A	117	ARG	CZ-NH1	-5.41	1.25	1.32	18	2
1	A	72	HIS	CG-ND1	-5.41	1.32	1.38	2	1
1	A	131	THR	N-CA	5.40	1.52	1.46	2	2
1	A	94	SER	C-O	5.40	1.30	1.24	13	1
1	A	30	ILE	N-CA	5.36	1.52	1.45	19	1
1	A	31	ASN	CA-C	5.36	1.60	1.52	14	1
1	A	47	THR	N-CA	5.36	1.52	1.45	13	1
1	A	102	PRO	N-CD	-5.35	1.40	1.47	8	2
1	A	46	THR	N-CA	5.35	1.52	1.45	1	1
1	A	74	SER	CA-C	5.34	1.59	1.52	2	1
1	A	87	ASN	C-O	-5.34	1.17	1.24	18	1
1	A	17	SER	C-N	5.33	1.40	1.33	18	1
1	A	129	LEU	CA-C	5.33	1.58	1.52	1	2
1	A	4	GLN	C-N	5.32	1.39	1.33	8	1
1	A	64	HIS	N-CA	5.31	1.55	1.46	18	1
1	A	107	TYR	C-O	5.31	1.30	1.23	5	1
1	A	70	ASN	C-O	5.31	1.30	1.23	14	1
1	A	61	ARG	NE-CZ	-5.31	1.27	1.33	3	1
1	A	100	ASP	N-CA	5.30	1.52	1.45	20	2
1	A	63	PRO	N-CA	5.30	1.53	1.47	15	1
1	A	47	THR	C-O	-5.30	1.17	1.23	16	1
1	A	106	PHE	C-O	-5.29	1.16	1.23	17	1
1	A	54	VAL	C-N	5.29	1.40	1.33	12	1
1	A	3	PRO	C-N	5.29	1.41	1.33	4	1
1	A	35	TRP	N-CA	-5.28	1.39	1.46	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	PHE	CA-CB	5.28	1.61	1.53	7	1
1	A	101	ARG	C-N	5.28	1.40	1.33	4	1
1	A	121	ARG	CD-NE	5.28	1.53	1.46	10	1
1	A	20	PRO	CA-CB	5.27	1.59	1.54	3	1
1	A	11	PHE	CA-C	5.27	1.59	1.52	4	1
1	A	51	VAL	CA-CB	-5.26	1.48	1.54	5	1
1	A	40	GLN	N-CA	5.26	1.52	1.45	17	1
1	A	126	PRO	CA-CB	5.25	1.60	1.53	12	1
1	A	133	ILE	CB-CG1	5.25	1.64	1.53	16	1
1	A	66	ARG	CZ-NH1	-5.25	1.25	1.32	20	1
1	A	30	ILE	C-O	-5.25	1.19	1.24	9	1
1	A	39	ASN	CA-C	5.25	1.59	1.52	19	1
1	A	38	LYS	CA-C	5.24	1.60	1.52	10	2
1	A	73	ARG	CD-NE	-5.24	1.39	1.46	11	1
1	A	44	LEU	C-N	5.23	1.40	1.33	18	1
1	A	45	ARG	N-CA	-5.23	1.40	1.46	20	1
1	A	73	ARG	CZ-NH2	-5.23	1.26	1.33	17	1
1	A	28	ARG	N-CA	5.23	1.52	1.46	18	2
1	A	107	TYR	N-CA	5.22	1.52	1.45	10	1
1	A	93	ILE	N-CA	5.22	1.52	1.46	20	1
1	A	89	GLY	C-N	5.21	1.40	1.33	7	1
1	A	43	PHE	CA-CB	5.21	1.61	1.53	13	1
1	A	68	LEU	N-CA	5.21	1.52	1.46	8	2
1	A	109	VAL	CA-C	5.21	1.59	1.52	15	1
1	A	28	ARG	CD-NE	5.18	1.53	1.46	1	1
1	A	34	ARG	CZ-NH1	-5.17	1.25	1.32	10	1
1	A	121	ARG	CZ-NH1	-5.17	1.25	1.32	19	1
1	A	69	ASN	C-O	-5.15	1.17	1.23	5	1
1	A	27	MET	CA-CB	5.15	1.62	1.53	18	1
1	A	86	ILE	C-N	5.14	1.37	1.33	1	1
1	A	26	ALA	CA-CB	5.13	1.61	1.53	17	1
1	A	48	PHE	CA-C	5.12	1.59	1.52	5	1
1	A	55	CYS	N-CA	-5.12	1.40	1.46	1	1
1	A	114	ARG	CA-CB	5.12	1.61	1.53	11	1
1	A	132	THR	C-N	5.11	1.40	1.33	14	1
1	A	27	MET	C-N	5.11	1.40	1.34	16	1
1	A	99	ALA	CA-C	5.10	1.58	1.52	1	1
1	A	10	TRP	CA-CB	5.09	1.62	1.53	11	1
1	A	19	ASN	N-CA	5.08	1.52	1.46	18	1
1	A	11	PHE	N-CA	5.08	1.52	1.46	2	1
1	A	121	ARG	CA-C	5.07	1.59	1.52	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	104	ARG	CA-CB	5.07	1.60	1.52	14	1
1	A	7	ARG	CZ-NH1	-5.07	1.25	1.32	9	1
1	A	100	ASP	CA-CB	-5.07	1.46	1.53	19	2
1	A	105	ARG	C-N	-5.06	1.27	1.33	3	1
1	A	117	ARG	NE-CZ	-5.05	1.27	1.33	11	1
1	A	59	SER	CA-CB	-5.05	1.45	1.53	4	1
1	A	113	ASN	N-CA	5.04	1.52	1.46	13	2
1	A	23	CYS	C-N	5.04	1.40	1.33	8	1
1	A	66	ARG	NE-CZ	-5.04	1.27	1.33	14	1
1	A	66	ARG	C-O	-5.03	1.18	1.24	8	1
1	A	129	LEU	N-CA	5.02	1.52	1.46	12	1
1	A	10	TRP	C-N	-5.01	1.27	1.33	19	1
1	A	7	ARG	C-O	-5.01	1.18	1.24	19	1
1	A	7	ARG	CD-NE	5.01	1.53	1.46	2	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLN	OE1-CD-NE2	-13.85	108.75	122.60	13	8
1	A	106	PHE	CA-CB-CG	13.30	127.10	113.80	2	5
1	A	20	PRO	O-C-N	11.93	126.76	121.15	13	1
1	A	87	ASN	OD1-CG-ND2	-11.90	110.70	122.60	14	11
1	A	19	ASN	CA-CB-CG	11.87	124.47	112.60	7	7
1	A	39	ASN	OD1-CG-ND2	-11.44	111.16	122.60	3	8
1	A	95	ASN	OD1-CG-ND2	-11.37	111.23	122.60	19	8
1	A	77	ARG	NE-CZ-NH1	11.15	132.65	121.50	5	3
1	A	34	ARG	NE-CZ-NH1	11.14	132.64	121.50	13	3
1	A	69	ASN	OD1-CG-ND2	-11.07	111.53	122.60	6	6
1	A	78	VAL	O-C-N	10.99	128.61	121.69	20	2
1	A	19	ASN	OD1-CG-ND2	-10.94	111.66	122.60	16	3
1	A	119	SER	CB-CA-C	10.47	118.64	111.20	20	3
1	A	112	ASP	CA-CB-CG	10.38	122.98	112.60	14	5
1	A	31	ASN	OD1-CG-ND2	-10.27	112.33	122.60	11	6
1	A	46	THR	CA-CB-OG1	10.26	124.98	109.60	6	2
1	A	62	CYS	O-C-N	-10.22	113.78	121.14	15	3
1	A	105	ARG	NE-CZ-NH1	10.11	131.61	121.50	17	3
1	A	117	ARG	NH1-CZ-NH2	-10.11	106.16	119.30	7	2
1	A	65	ASN	OD1-CG-ND2	-10.04	112.56	122.60	1	3
1	A	87	ASN	CA-C-N	10.03	131.10	119.47	2	9
1	A	87	ASN	C-N-CA	10.03	131.10	119.47	2	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	ASN	CA-CB-CG	9.80	122.40	112.60	15	6
1	A	19	ASN	CA-C-N	9.76	130.44	120.38	18	6
1	A	19	ASN	C-N-CA	9.76	130.44	120.38	18	6
1	A	38	LYS	CA-C-N	9.76	133.36	120.28	13	9
1	A	38	LYS	C-N-CA	9.76	133.36	120.28	13	9
1	A	39	ASN	N-CA-C	9.61	121.52	111.14	20	5
1	A	2	PRO	CA-C-N	9.60	129.84	119.28	16	9
1	A	2	PRO	C-N-CA	9.60	129.84	119.28	16	9
1	A	84	ASP	CA-CB-CG	9.58	122.18	112.60	11	5
1	A	10	TRP	N-CA-C	9.53	121.67	111.28	3	4
1	A	40	GLN	OE1-CD-NE2	-9.43	113.17	122.60	17	4
1	A	77	ARG	NE-CZ-NH2	9.43	127.69	119.20	9	4
1	A	77	ARG	NH1-CZ-NH2	-9.40	107.08	119.30	1	4
1	A	97	ARG	NE-CZ-NH1	9.36	130.86	121.50	2	3
1	A	64	HIS	CA-CB-CG	9.35	123.15	113.80	14	7
1	A	70	ASN	OD1-CG-ND2	-9.32	113.28	122.60	19	5
1	A	15	HIS	CB-CG-CD2	-9.26	119.16	131.20	1	7
1	A	35	TRP	N-CA-C	9.25	122.34	111.71	20	5
1	A	76	PHE	CA-CB-CG	9.23	123.03	113.80	7	5
1	A	7	ARG	CA-C-N	9.21	133.55	120.28	14	4
1	A	7	ARG	C-N-CA	9.21	133.55	120.28	14	4
1	A	50	ASN	OD1-CG-ND2	-9.21	113.39	122.60	3	5
1	A	72	HIS	CB-CG-CD2	-9.13	119.33	131.20	4	7
1	A	114	ARG	NE-CZ-NH2	9.09	127.38	119.20	12	3
1	A	53	ASN	OD1-CG-ND2	-8.97	113.63	122.60	1	6
1	A	117	ARG	NE-CZ-NH1	8.97	130.47	121.50	7	4
1	A	101	ARG	CA-C-N	8.92	128.99	119.90	20	7
1	A	101	ARG	C-N-CA	8.92	128.99	119.90	20	7
1	A	2	PRO	N-CA-CB	8.76	111.58	103.08	13	4
1	A	31	ASN	CA-CB-CG	8.74	121.34	112.60	12	2
1	A	79	PRO	O-C-N	-8.72	112.25	122.71	1	2
1	A	7	ARG	CA-C-O	-8.66	111.72	120.82	5	2
1	A	126	PRO	CA-C-N	8.66	133.65	121.53	16	1
1	A	126	PRO	C-N-CA	8.66	133.65	121.53	16	1
1	A	113	ASN	OD1-CG-ND2	-8.62	113.98	122.60	4	2
1	A	23	CYS	CA-C-N	8.58	132.63	120.28	19	4
1	A	23	CYS	C-N-CA	8.58	132.63	120.28	19	4
1	A	2	PRO	N-CA-C	8.55	121.14	110.70	2	4
1	A	3	PRO	N-CA-CB	8.52	112.00	103.48	3	4
1	A	49	ALA	CA-C-O	-8.43	111.53	120.63	1	2
1	A	121	ARG	NE-CZ-NH2	8.39	126.75	119.20	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	43	PHE	CA-CB-CG	8.38	122.18	113.80	7	3
1	A	80	LEU	CA-C-N	8.33	134.34	121.76	12	2
1	A	80	LEU	C-N-CA	8.33	134.34	121.76	12	2
1	A	57	ASN	OD1-CG-ND2	-8.33	114.27	122.60	10	5
1	A	58	GLN	OE1-CD-NE2	-8.32	114.28	122.60	6	5
1	A	20	PRO	CA-C-N	8.26	130.17	119.84	8	3
1	A	20	PRO	C-N-CA	8.26	130.17	119.84	8	3
1	A	28	ARG	NE-CZ-NH1	8.23	129.73	121.50	8	2
1	A	32	ASN	OD1-CG-ND2	-8.23	114.37	122.60	19	5
1	A	93	ILE	CA-CB-CG1	8.22	124.37	110.40	12	1
1	A	48	PHE	O-C-N	8.21	130.63	122.09	12	1
1	A	61	ARG	NH1-CZ-NH2	-8.21	108.63	119.30	6	1
1	A	82	HIS	CB-CG-CD2	-8.20	120.55	131.20	4	5
1	A	32	ASN	CA-CB-CG	8.18	120.78	112.60	20	6
1	A	125	VAL	CA-C-N	8.18	128.11	119.85	20	7
1	A	125	VAL	C-N-CA	8.18	128.11	119.85	20	7
1	A	61	ARG	NE-CZ-NH1	8.17	129.67	121.50	3	4
1	A	34	ARG	NE-CZ-NH2	8.17	126.55	119.20	3	5
1	A	9	GLN	OE1-CD-NE2	-8.12	114.48	122.60	14	9
1	A	7	ARG	NE-CZ-NH2	-8.11	111.90	119.20	20	2
1	A	76	PHE	CA-C-O	-8.10	112.44	121.51	6	2
1	A	93	ILE	CA-C-N	8.10	131.13	120.28	19	2
1	A	93	ILE	C-N-CA	8.10	131.13	120.28	19	2
1	A	64	HIS	CB-CG-CD2	-8.08	120.69	131.20	10	7
1	A	116	PRO	N-CA-CB	8.07	112.34	103.30	19	1
1	A	11	PHE	CA-C-N	8.05	131.98	120.79	17	3
1	A	11	PHE	C-N-CA	8.05	131.98	120.79	17	3
1	A	34	ARG	NH1-CZ-NH2	-8.05	108.84	119.30	2	2
1	A	92	ASN	CA-CB-CG	8.03	120.63	112.60	20	3
1	A	63	PRO	N-CA-C	8.02	124.26	113.84	14	2
1	A	54	VAL	O-C-N	-8.01	113.58	121.83	18	1
1	A	4	GLN	OE1-CD-NE2	-8.00	114.60	122.60	2	6
1	A	7	ARG	NE-CZ-NH1	8.00	129.50	121.50	20	4
1	A	91	GLN	O-C-N	-8.00	113.45	121.93	13	2
1	A	5	PHE	CA-CB-CG	-8.00	105.80	113.80	2	7
1	A	101	ARG	NE-CZ-NH2	-7.99	112.01	119.20	5	3
1	A	118	ASP	CA-C-N	7.97	131.44	122.83	18	1
1	A	118	ASP	C-N-CA	7.97	131.44	122.83	18	1
1	A	120	PRO	CA-C-N	7.96	135.80	120.99	13	3
1	A	120	PRO	C-N-CA	7.96	135.80	120.99	13	3
1	A	119	SER	CA-C-N	7.93	127.65	119.56	20	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	119	SER	C-N-CA	7.93	127.65	119.56	20	4
1	A	20	PRO	N-CA-CB	7.92	110.76	103.08	19	3
1	A	11	PHE	CA-CB-CG	-7.92	105.88	113.80	20	2
1	A	46	THR	CA-C-N	7.91	132.73	121.42	1	2
1	A	46	THR	C-N-CA	7.91	132.73	121.42	1	2
1	A	75	ARG	NE-CZ-NH1	7.91	129.41	121.50	16	3
1	A	62	CYS	CA-C-N	7.90	127.62	119.56	7	3
1	A	62	CYS	C-N-CA	7.90	127.62	119.56	7	3
1	A	25	ILE	CB-CA-C	-7.89	103.18	110.91	15	2
1	A	25	ILE	N-CA-C	-7.87	105.51	112.12	12	2
1	A	82	HIS	CB-CG-ND1	7.83	134.44	122.70	4	1
1	A	15	HIS	N-CA-C	7.82	125.73	114.16	19	1
1	A	87	ASN	CA-CB-CG	-7.78	104.82	112.60	2	3
1	A	115	ASP	N-CA-CB	-7.76	98.87	110.05	19	1
1	A	77	ARG	CA-C-O	-7.72	113.15	121.56	2	1
1	A	66	ARG	NE-CZ-NH2	7.67	126.10	119.20	16	2
1	A	30	ILE	CA-C-O	-7.66	111.21	120.78	13	2
1	A	63	PRO	N-CA-CB	7.65	111.33	102.76	17	3
1	A	102	PRO	N-CA-CB	7.63	109.97	103.25	20	2
1	A	105	ARG	CA-C-O	-7.62	112.79	121.40	2	1
1	A	115	ASP	CA-CB-CG	7.61	120.21	112.60	18	4
1	A	119	SER	CA-C-O	-7.60	114.63	120.48	17	3
1	A	101	ARG	NE-CZ-NH1	7.59	129.09	121.50	4	5
1	A	97	ARG	NH1-CZ-NH2	-7.59	109.44	119.30	2	4
1	A	87	ASN	CB-CG-ND2	7.58	127.77	116.40	14	1
1	A	117	ARG	NE-CZ-NH2	7.56	126.00	119.20	17	6
1	A	52	VAL	O-C-N	-7.52	114.57	121.87	13	4
1	A	109	VAL	N-CA-CB	-7.51	104.04	112.45	7	1
1	A	106	PHE	N-CA-CB	-7.48	100.08	110.25	3	2
1	A	11	PHE	N-CA-C	7.46	120.07	111.11	18	1
1	A	101	ARG	CD-NE-CZ	7.46	134.84	124.40	9	2
1	A	58	GLN	O-C-N	-7.45	113.88	122.97	9	1
1	A	101	ARG	NH1-CZ-NH2	-7.45	109.61	119.30	11	2
1	A	70	ASN	CA-C-N	7.45	134.09	121.87	1	4
1	A	70	ASN	C-N-CA	7.45	134.09	121.87	1	4
1	A	53	ASN	CA-CB-CG	-7.44	105.16	112.60	5	5
1	A	45	ARG	NE-CZ-NH1	7.43	128.93	121.50	6	4
1	A	71	CYS	CA-C-N	7.43	134.25	122.21	16	2
1	A	71	CYS	C-N-CA	7.43	134.25	122.21	16	2
1	A	90	ALA	N-CA-CB	-7.39	98.84	109.85	8	1
1	A	75	ARG	N-CA-C	-7.36	104.17	113.01	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	THR	CA-CB-OG1	7.36	120.64	109.60	1	1
1	A	92	ASN	OD1-CG-ND2	-7.36	115.25	122.60	3	5
1	A	47	THR	CA-CB-OG1	7.35	120.63	109.60	17	4
1	A	22	ARG	NE-CZ-NH1	7.35	128.85	121.50	1	3
1	A	87	ASN	CB-CA-C	7.33	119.87	110.34	3	1
1	A	64	HIS	CA-C-O	7.33	127.62	121.02	3	1
1	A	105	ARG	NH1-CZ-NH2	-7.32	109.78	119.30	19	4
1	A	12	ALA	N-CA-C	7.31	119.89	111.11	13	3
1	A	122	TYR	O-C-N	7.29	127.87	121.39	9	2
1	A	16	ILE	O-C-N	7.28	129.77	122.71	5	1
1	A	119	SER	O-C-N	-7.27	118.18	121.53	16	1
1	A	102	PRO	CA-C-N	7.26	130.87	120.56	10	1
1	A	102	PRO	C-N-CA	7.26	130.87	120.56	10	1
1	A	75	ARG	CD-NE-CZ	7.26	134.56	124.40	2	3
1	A	132	THR	OG1-CB-CG2	-7.25	94.81	109.30	18	1
1	A	7	ARG	O-C-N	7.20	129.75	122.12	19	2
1	A	72	HIS	ND1-CE1-NE2	7.19	115.59	108.40	3	2
1	A	53	ASN	CA-C-O	-7.19	111.70	119.97	8	1
1	A	14	GLN	CA-C-O	-7.19	111.31	119.79	16	1
1	A	22	ARG	CD-NE-CZ	7.18	134.45	124.40	7	3
1	A	46	THR	CA-CB-CG2	7.17	122.68	110.50	17	2
1	A	42	THR	CA-C-N	7.16	133.28	123.11	14	4
1	A	42	THR	C-N-CA	7.16	133.28	123.11	14	4
1	A	51	VAL	CA-C-N	7.15	130.57	120.42	2	2
1	A	51	VAL	C-N-CA	7.15	130.57	120.42	2	2
1	A	86	ILE	CA-C-O	-7.15	112.92	120.57	8	2
1	A	86	ILE	CA-CB-CG1	7.14	122.54	110.40	13	3
1	A	73	ARG	NE-CZ-NH2	7.13	125.62	119.20	1	3
1	A	65	ASN	CA-C-N	7.13	132.12	120.63	14	4
1	A	65	ASN	C-N-CA	7.13	132.12	120.63	14	4
1	A	118	ASP	N-CA-CB	-7.12	99.31	111.69	8	1
1	A	74	SER	CA-CB-OG	7.11	125.31	111.10	18	1
1	A	3	PRO	N-CA-C	7.10	123.14	113.98	8	2
1	A	133	ILE	CA-CB-CG1	7.10	122.47	110.40	8	5
1	A	27	MET	O-C-N	-7.09	113.92	122.22	17	1
1	A	128	HIS	CA-CB-CG	7.09	120.89	113.80	15	3
1	A	117	ARG	CA-C-O	-7.09	110.47	118.55	11	2
1	A	15	HIS	O-C-N	-7.06	114.92	122.19	12	4
1	A	93	ILE	N-CA-C	7.04	117.76	110.36	20	3
1	A	15	HIS	CA-CB-CG	7.04	120.84	113.80	16	2
1	A	95	ASN	CB-CG-ND2	7.04	126.96	116.40	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	128	HIS	N-CA-C	7.03	119.76	109.07	15	1
1	A	25	ILE	CA-C-N	7.02	130.39	120.28	5	2
1	A	25	ILE	C-N-CA	7.02	130.39	120.28	5	2
1	A	105	ARG	NE-CZ-NH2	-7.01	112.89	119.20	7	5
1	A	61	ARG	NE-CZ-NH2	7.00	125.50	119.20	10	4
1	A	120	PRO	N-CA-C	6.99	126.86	112.47	6	2
1	A	105	ARG	CD-NE-CZ	6.98	134.18	124.40	2	2
1	A	72	HIS	CA-CB-CG	6.98	120.78	113.80	12	1
1	A	29	ALA	N-CA-C	6.98	121.41	112.34	16	1
1	A	113	ASN	CA-CB-CG	6.97	119.57	112.60	11	1
1	A	19	ASN	N-CA-CB	-6.94	102.86	110.71	12	1
1	A	123	PRO	CA-C-N	6.94	132.54	122.69	9	2
1	A	123	PRO	C-N-CA	6.94	132.54	122.69	9	2
1	A	23	CYS	N-CA-C	6.93	119.69	111.71	9	3
1	A	22	ARG	NE-CZ-NH2	6.93	125.44	119.20	11	5
1	A	104	ARG	NE-CZ-NH1	6.93	128.43	121.50	2	3
1	A	52	VAL	CA-C-O	-6.91	113.52	120.85	10	2
1	A	85	LEU	CD1-CG-CD2	-6.91	95.59	110.80	2	1
1	A	65	ASN	CB-CG-ND2	6.91	126.76	116.40	1	2
1	A	59	SER	CA-C-O	-6.88	112.72	120.43	18	2
1	A	80	LEU	N-CA-C	6.86	117.64	108.38	1	4
1	A	75	ARG	NE-CZ-NH2	-6.86	113.03	119.20	16	2
1	A	5	PHE	N-CA-C	6.84	119.16	108.96	12	1
1	A	122	TYR	CA-C-N	6.84	126.55	119.64	4	4
1	A	122	TYR	C-N-CA	6.84	126.55	119.64	4	4
1	A	18	LEU	CA-C-N	6.83	128.29	122.28	17	3
1	A	18	LEU	C-N-CA	6.83	128.29	122.28	17	3
1	A	85	LEU	CA-C-O	-6.83	113.61	120.98	5	1
1	A	132	THR	CA-CB-CG2	6.83	122.10	110.50	8	4
1	A	118	ASP	N-CA-C	6.82	119.54	109.24	8	1
1	A	88	PRO	CA-C-O	-6.81	108.88	119.64	19	1
1	A	39	ASN	N-CA-CB	-6.80	100.12	110.12	1	2
1	A	128	HIS	CB-CG-CD2	-6.79	122.37	131.20	14	5
1	A	97	ARG	CD-NE-CZ	6.79	133.91	124.40	9	1
1	A	67	THR	CA-CB-OG1	-6.78	99.44	109.60	13	4
1	A	77	ARG	N-CA-C	6.77	118.74	110.41	20	1
1	A	100	ASP	CA-C-N	6.77	128.24	122.28	8	2
1	A	100	ASP	C-N-CA	6.77	128.24	122.28	8	2
1	A	4	GLN	CB-CA-C	6.76	120.78	110.37	15	1
1	A	73	ARG	NH1-CZ-NH2	-6.74	110.54	119.30	1	2
1	A	90	ALA	N-CA-C	6.73	120.44	110.48	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	79	PRO	CA-C-N	6.72	134.11	122.82	9	2
1	A	79	PRO	C-N-CA	6.72	134.11	122.82	9	2
1	A	71	CYS	O-C-N	-6.72	115.59	123.25	4	1
1	A	68	LEU	CA-C-N	6.71	131.67	122.07	2	3
1	A	68	LEU	C-N-CA	6.71	131.67	122.07	2	3
1	A	28	ARG	CA-C-O	-6.71	112.52	120.10	18	1
1	A	103	GLY	O-C-N	-6.71	117.48	123.92	3	1
1	A	129	LEU	CA-C-O	-6.70	112.04	120.28	10	4
1	A	25	ILE	CA-C-O	-6.69	114.25	120.34	12	3
1	A	58	GLN	CA-C-O	-6.69	114.46	121.55	15	2
1	A	114	ARG	N-CA-C	6.69	119.67	110.24	6	3
1	A	66	ARG	O-C-N	6.69	129.21	122.12	6	1
1	A	25	ILE	CA-CB-CG1	6.68	121.76	110.40	16	3
1	A	69	ASN	CA-CB-CG	6.68	119.28	112.60	6	3
1	A	131	THR	CA-C-N	6.68	133.69	121.94	7	4
1	A	131	THR	C-N-CA	6.68	133.69	121.94	7	4
1	A	130	ASP	CA-C-O	6.67	127.62	119.81	2	1
1	A	6	THR	CA-CB-CG2	6.67	121.84	110.50	16	3
1	A	113	ASN	CA-C-N	6.67	131.25	121.31	14	3
1	A	113	ASN	C-N-CA	6.67	131.25	121.31	14	3
1	A	13	ILE	CA-C-O	-6.66	113.45	120.57	1	2
1	A	88	PRO	N-CA-CB	6.66	110.75	103.30	3	3
1	A	38	LYS	O-C-N	-6.65	114.75	122.93	13	1
1	A	92	ASN	O-C-N	-6.65	114.79	123.16	2	3
1	A	75	ARG	NH1-CZ-NH2	-6.64	110.66	119.30	15	1
1	A	95	ASN	CA-C-N	6.63	130.53	121.05	16	3
1	A	95	ASN	C-N-CA	6.63	130.53	121.05	16	3
1	A	19	ASN	O-C-N	6.61	126.76	121.20	2	5
1	A	107	TYR	CA-C-N	6.61	132.81	122.70	15	2
1	A	107	TYR	C-N-CA	6.61	132.81	122.70	15	2
1	A	115	ASP	O-C-N	-6.60	115.04	121.18	4	1
1	A	41	ASN	OD1-CG-ND2	-6.60	116.00	122.60	6	2
1	A	10	TRP	CB-CG-CD2	6.60	136.04	126.80	16	2
1	A	16	ILE	N-CA-C	6.58	118.30	107.24	14	1
1	A	66	ARG	N-CA-C	6.58	120.90	112.34	7	3
1	A	95	ASN	CA-CB-CG	6.58	119.18	112.60	11	3
1	A	17	SER	CA-C-N	6.57	129.38	120.38	10	4
1	A	17	SER	C-N-CA	6.57	129.38	120.38	10	4
1	A	104	ARG	O-C-N	6.57	131.41	123.26	10	1
1	A	15	HIS	CB-CG-ND1	6.56	132.54	122.70	1	1
1	A	117	ARG	CD-NE-CZ	6.56	133.58	124.40	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	ARG	NH1-CZ-NH2	-6.55	110.78	119.30	15	3
1	A	45	ARG	NE-CZ-NH2	-6.55	113.31	119.20	13	5
1	A	106	PHE	O-C-N	-6.54	114.67	122.65	4	1
1	A	57	ASN	CA-CB-CG	6.54	119.14	112.60	13	4
1	A	125	VAL	O-C-N	6.53	128.55	121.10	15	2
1	A	14	GLN	OE1-CD-NE2	-6.53	116.07	122.60	7	5
1	A	89	GLY	CA-C-N	6.53	130.02	120.82	2	1
1	A	89	GLY	C-N-CA	6.53	130.02	120.82	2	1
1	A	131	THR	CA-C-O	6.52	128.43	121.45	16	1
1	A	30	ILE	N-CA-C	6.51	119.47	112.96	9	1
1	A	107	TYR	CG-CD1-CE1	-6.50	111.44	121.20	19	1
1	A	69	ASN	CA-C-N	6.49	131.99	122.39	19	1
1	A	69	ASN	C-N-CA	6.49	131.99	122.39	19	1
1	A	62	CYS	CA-C-O	-6.48	114.22	120.64	9	1
1	A	80	LEU	CA-C-O	6.48	128.38	121.45	11	2
1	A	84	ASP	N-CA-CB	-6.47	101.13	111.62	6	3
1	A	10	TRP	CE2-CD2-CE3	-6.46	112.34	118.80	20	2
1	A	60	ILE	O-C-N	-6.45	115.91	122.75	2	3
1	A	31	ASN	CB-CG-ND2	6.45	126.08	116.40	5	1
1	A	41	ASN	CA-CB-CG	-6.45	106.15	112.60	2	3
1	A	111	CYS	N-CA-C	6.45	119.52	109.52	6	2
1	A	46	THR	CA-C-O	-6.45	114.37	121.33	7	1
1	A	128	HIS	CG-CD2-NE2	-6.44	100.76	107.20	18	2
1	A	28	ARG	CA-C-N	6.43	129.76	120.38	6	2
1	A	28	ARG	C-N-CA	6.43	129.76	120.38	6	2
1	A	30	ILE	CB-CA-C	6.43	117.17	111.71	15	1
1	A	55	CYS	CA-C-N	6.42	128.43	120.34	3	2
1	A	55	CYS	C-N-CA	6.42	128.43	120.34	3	2
1	A	48	PHE	CA-C-N	6.41	129.20	120.54	20	1
1	A	48	PHE	C-N-CA	6.41	129.20	120.54	20	1
1	A	45	ARG	NH1-CZ-NH2	-6.41	110.97	119.30	5	3
1	A	131	THR	CA-CB-CG2	6.40	121.38	110.50	14	4
1	A	51	VAL	N-CA-C	-6.40	104.02	111.00	7	2
1	A	78	VAL	CA-C-N	6.40	126.35	119.76	9	1
1	A	78	VAL	C-N-CA	6.40	126.35	119.76	9	1
1	A	50	ASN	CA-CB-CG	-6.40	106.20	112.60	8	2
1	A	102	PRO	N-CA-C	6.40	120.48	111.33	13	1
1	A	57	ASN	N-CA-C	6.39	118.80	110.43	20	3
1	A	4	GLN	N-CA-C	6.39	122.15	113.21	17	1
1	A	5	PHE	CA-C-O	6.36	128.59	121.40	5	1
1	A	62	CYS	N-CA-C	6.36	118.53	108.23	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	ASN	CB-CG-ND2	6.35	125.93	116.40	12	1
1	A	95	ASN	N-CA-C	-6.35	105.43	113.43	8	1
1	A	114	ARG	CA-C-N	6.34	129.90	120.83	8	1
1	A	114	ARG	C-N-CA	6.34	129.90	120.83	8	1
1	A	24	THR	N-CA-C	6.33	119.86	111.75	13	2
1	A	35	TRP	NE1-CE2-CD2	-6.33	99.18	107.40	20	1
1	A	130	ASP	CA-CB-CG	6.32	118.92	112.60	11	2
1	A	35	TRP	CE2-CD2-CE3	-6.32	112.48	118.80	20	1
1	A	126	PRO	N-CA-CB	6.31	108.92	103.31	19	2
1	A	96	CYS	CB-CA-C	6.30	120.43	109.65	12	2
1	A	68	LEU	CB-CA-C	6.30	117.29	109.16	1	2
1	A	72	HIS	ND1-CG-CD2	6.29	112.39	106.10	16	4
1	A	103	GLY	CA-C-N	6.28	130.13	121.33	18	3
1	A	103	GLY	C-N-CA	6.28	130.13	121.33	18	3
1	A	59	SER	CA-C-N	6.28	131.96	122.92	11	3
1	A	59	SER	C-N-CA	6.28	131.96	122.92	11	3
1	A	52	VAL	CA-CB-CG1	6.28	121.07	110.40	1	2
1	A	102	PRO	CB-CA-C	6.25	119.50	111.56	20	2
1	A	98	TYR	N-CA-C	6.25	117.68	108.86	3	1
1	A	27	MET	CA-C-N	6.25	129.28	120.28	6	2
1	A	27	MET	C-N-CA	6.25	129.28	120.28	6	2
1	A	124	VAL	N-CA-C	-6.25	99.49	108.42	6	1
1	A	28	ARG	NH1-CZ-NH2	-6.24	111.18	119.30	8	2
1	A	65	ASN	N-CA-CB	-6.24	101.12	111.49	10	2
1	A	14	GLN	CG-CD-NE2	6.23	125.74	116.40	4	1
1	A	64	HIS	O-C-N	-6.22	114.32	122.59	4	1
1	A	51	VAL	CA-CB-CG2	6.21	120.96	110.40	1	3
1	A	36	ARG	CA-C-N	6.21	130.21	121.02	5	3
1	A	36	ARG	C-N-CA	6.21	130.21	121.02	5	3
1	A	92	ASN	CA-C-N	6.21	129.28	120.53	4	3
1	A	92	ASN	C-N-CA	6.21	129.28	120.53	4	3
1	A	127	VAL	CA-CB-CG2	6.20	120.94	110.40	10	3
1	A	35	TRP	CA-C-N	6.19	132.23	122.21	1	3
1	A	35	TRP	C-N-CA	6.19	132.23	122.21	1	3
1	A	54	VAL	CA-CB-CG1	6.17	120.88	110.40	19	2
1	A	122	TYR	CB-CA-C	6.16	118.35	110.34	2	2
1	A	72	HIS	CA-C-O	-6.16	114.86	121.45	10	3
1	A	81	LEU	CB-CA-C	6.16	120.83	110.79	6	1
1	A	45	ARG	CD-NE-CZ	6.16	133.02	124.40	14	1
1	A	58	GLN	CA-C-N	6.15	130.12	121.02	13	1
1	A	58	GLN	C-N-CA	6.15	130.12	121.02	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	ALA	CA-C-O	-6.15	114.37	120.70	9	2
1	A	17	SER	O-C-N	6.15	131.35	123.24	18	1
1	A	39	ASN	CA-C-N	6.14	132.72	121.85	5	1
1	A	39	ASN	C-N-CA	6.14	132.72	121.85	5	1
1	A	14	GLN	N-CA-C	6.14	120.61	113.18	14	1
1	A	61	ARG	CD-NE-CZ	6.14	132.99	124.40	12	1
1	A	84	ASP	CA-C-N	6.13	131.41	122.77	6	1
1	A	84	ASP	C-N-CA	6.13	131.41	122.77	6	1
1	A	65	ASN	O-C-N	-6.12	115.41	122.09	12	1
1	A	13	ILE	CA-CB-CG2	6.12	120.91	110.50	5	2
1	A	41	ASN	CA-C-N	6.11	132.63	122.73	17	1
1	A	41	ASN	C-N-CA	6.11	132.63	122.73	17	1
1	A	114	ARG	N-CA-CB	6.11	118.60	109.19	8	1
1	A	97	ARG	NE-CZ-NH2	6.11	124.70	119.20	12	2
1	A	95	ASN	N-CA-CB	-6.11	101.55	110.47	19	1
1	A	31	ASN	CA-C-O	6.11	126.42	119.27	10	1
1	A	37	CYS	CA-C-O	-6.11	113.64	120.54	11	1
1	A	18	LEU	O-C-N	6.10	129.58	122.20	11	1
1	A	75	ARG	CA-C-N	6.08	132.33	122.29	20	4
1	A	75	ARG	C-N-CA	6.08	132.33	122.29	20	4
1	A	3	PRO	CA-C-N	6.08	129.57	119.35	17	1
1	A	3	PRO	C-N-CA	6.08	129.57	119.35	17	1
1	A	132	THR	CA-C-N	6.08	132.65	121.70	7	1
1	A	132	THR	C-N-CA	6.08	132.65	121.70	7	1
1	A	10	TRP	NE1-CE2-CD2	-6.08	99.50	107.40	3	1
1	A	47	THR	CA-C-O	-6.08	114.12	121.05	1	3
1	A	41	ASN	CA-C-O	-6.08	114.95	121.45	19	1
1	A	3	PRO	N-CD-CG	6.07	112.30	103.20	11	1
1	A	47	THR	CA-C-N	6.07	128.69	120.38	10	3
1	A	47	THR	C-N-CA	6.07	128.69	120.38	10	3
1	A	36	ARG	NE-CZ-NH2	6.07	124.66	119.20	20	1
1	A	66	ARG	CA-C-N	6.07	128.69	120.38	15	1
1	A	66	ARG	C-N-CA	6.07	128.69	120.38	15	1
1	A	82	HIS	ND1-CG-CD2	6.06	112.16	106.10	11	1
1	A	95	ASN	O-C-N	6.05	129.39	122.25	6	1
1	A	46	THR	OG1-CB-CG2	-6.05	97.20	109.30	15	1
1	A	127	VAL	O-C-N	-6.05	115.01	122.57	9	2
1	A	52	VAL	CA-C-N	6.03	128.64	120.44	5	1
1	A	52	VAL	C-N-CA	6.03	128.64	120.44	5	1
1	A	50	ASN	CA-C-N	6.03	130.66	120.29	9	2
1	A	50	ASN	C-N-CA	6.03	130.66	120.29	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	ASN	CA-C-O	6.03	126.81	120.42	14	3
1	A	99	ALA	O-C-N	-6.02	116.55	123.42	17	3
1	A	3	PRO	CA-N-CD	-6.02	103.57	112.00	11	2
1	A	117	ARG	N-CA-CB	-6.01	101.51	111.49	20	1
1	A	114	ARG	CA-C-O	-6.01	114.58	121.07	14	2
1	A	130	ASP	CA-C-N	6.01	132.07	121.80	11	1
1	A	130	ASP	C-N-CA	6.01	132.07	121.80	11	1
1	A	115	ASP	N-CA-C	6.00	118.18	109.84	2	3
1	A	114	ARG	CD-NE-CZ	6.00	132.79	124.40	17	1
1	A	57	ASN	N-CA-CB	-6.00	101.69	110.26	20	2
1	A	82	HIS	ND1-CE1-NE2	5.99	114.39	108.40	18	1
1	A	33	TYR	CB-CA-C	5.98	118.33	109.29	7	1
1	A	43	PHE	N-CA-CB	-5.98	100.85	111.08	20	1
1	A	11	PHE	CA-C-O	5.98	127.30	120.90	7	2
1	A	103	GLY	N-CA-C	5.97	120.34	110.55	4	2
1	A	65	ASN	CA-C-O	5.97	125.09	118.52	14	1
1	A	100	ASP	CA-CB-CG	5.96	118.56	112.60	13	2
1	A	79	PRO	CB-CA-C	5.96	118.76	110.95	15	2
1	A	87	ASN	N-CA-CB	-5.96	103.59	111.40	17	1
1	A	89	GLY	O-C-N	-5.95	114.96	122.70	1	2
1	A	90	ALA	CB-CA-C	5.95	119.60	109.72	7	1
1	A	98	TYR	CA-C-O	5.95	128.17	121.51	13	1
1	A	93	ILE	O-C-N	-5.95	114.85	122.22	15	3
1	A	100	ASP	N-CA-C	5.95	119.28	110.48	3	1
1	A	13	ILE	N-CA-C	5.93	116.11	110.42	9	1
1	A	11	PHE	CD1-CG-CD2	5.93	127.49	118.60	12	1
1	A	108	VAL	CB-CA-C	-5.92	103.68	110.73	18	1
1	A	61	ARG	CA-C-N	5.92	134.46	122.45	13	1
1	A	61	ARG	C-N-CA	5.92	134.46	122.45	13	1
1	A	72	HIS	CB-CG-ND1	5.91	131.56	122.70	6	3
1	A	107	TYR	CB-CG-CD1	5.90	129.65	120.80	12	1
1	A	10	TRP	CG-CD2-CE3	5.89	139.79	133.90	20	1
1	A	45	ARG	N-CA-CB	5.89	120.44	110.49	1	1
1	A	7	ARG	CA-CB-CG	-5.89	102.32	114.10	3	2
1	A	77	ARG	CB-CA-C	-5.89	99.53	109.83	14	1
1	A	70	ASN	O-C-N	-5.88	116.20	123.44	4	1
1	A	113	ASN	CA-C-O	-5.88	114.68	121.15	12	3
1	A	18	LEU	N-CA-CB	-5.88	101.17	110.28	15	1
1	A	33	TYR	N-CA-CB	-5.88	99.90	111.60	17	1
1	A	92	ASN	N-CA-CB	-5.87	101.36	110.57	9	1
1	A	18	LEU	N-CA-C	5.86	118.62	111.82	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	ARG	CB-CG-CD	5.86	124.79	111.30	5	1
1	A	51	VAL	CB-CA-C	-5.86	104.38	112.24	12	1
1	A	21	PRO	O-C-N	-5.86	115.59	122.86	20	2
1	A	66	ARG	NE-CZ-NH1	5.85	127.35	121.50	2	2
1	A	19	ASN	CB-CA-C	5.85	118.40	111.15	12	1
1	A	5	PHE	CG-CD1-CE1	-5.85	110.76	120.70	19	1
1	A	98	TYR	CA-CB-CG	5.83	124.39	113.90	8	1
1	A	76	PHE	O-C-N	-5.83	117.14	123.26	11	1
1	A	100	ASP	CA-C-O	-5.82	114.38	121.36	1	2
1	A	32	ASN	CA-C-N	5.81	132.31	122.26	19	2
1	A	32	ASN	C-N-CA	5.81	132.31	122.26	19	2
1	A	104	ARG	CA-C-N	5.81	131.80	121.75	12	1
1	A	104	ARG	C-N-CA	5.81	131.80	121.75	12	1
1	A	104	ARG	CB-CA-C	5.81	118.72	110.24	3	3
1	A	36	ARG	CD-NE-CZ	5.81	132.53	124.40	16	2
1	A	4	GLN	CA-C-O	-5.80	113.02	119.34	11	1
1	A	127	VAL	CA-C-N	5.79	131.78	121.75	15	2
1	A	127	VAL	C-N-CA	5.79	131.78	121.75	15	2
1	A	82	HIS	CB-CA-C	5.78	120.72	109.33	13	3
1	A	117	ARG	CA-C-N	5.78	129.68	121.42	19	1
1	A	117	ARG	C-N-CA	5.78	129.68	121.42	19	1
1	A	66	ARG	CD-NE-CZ	5.78	132.49	124.40	8	2
1	A	48	PHE	CA-C-O	-5.77	114.40	120.63	4	1
1	A	83	CYS	N-CA-CB	-5.77	101.86	111.20	18	2
1	A	24	THR	CA-CB-OG1	-5.76	100.96	109.60	6	1
1	A	104	ARG	CA-C-O	5.76	127.51	120.25	1	3
1	A	98	TYR	N-CA-CB	-5.76	101.70	111.31	1	1
1	A	18	LEU	CA-C-O	-5.75	114.46	120.55	16	1
1	A	121	ARG	N-CA-C	5.74	119.81	112.34	11	3
1	A	26	ALA	CA-C-O	5.72	126.49	120.42	2	3
1	A	38	LYS	N-CA-C	-5.72	101.81	110.28	6	1
1	A	108	VAL	O-C-N	-5.72	117.14	123.03	17	1
1	A	121	ARG	NH1-CZ-NH2	-5.72	111.86	119.30	13	1
1	A	24	THR	CA-C-N	5.72	128.78	122.77	19	1
1	A	24	THR	C-N-CA	5.72	128.78	122.77	19	1
1	A	121	ARG	NE-CZ-NH1	5.71	127.21	121.50	7	1
1	A	7	ARG	CB-CG-CD	5.70	124.41	111.30	3	2
1	A	127	VAL	N-CA-C	5.70	119.22	113.47	6	2
1	A	107	TYR	CD1-CG-CD2	5.70	126.64	118.10	19	1
1	A	42	THR	CA-CB-CG2	5.69	120.18	110.50	14	4
1	A	40	GLN	O-C-N	-5.69	116.67	123.27	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	GLN	CA-C-O	5.69	126.79	120.82	19	1
1	A	73	ARG	CD-NE-CZ	5.68	132.36	124.40	3	1
1	A	66	ARG	CA-C-O	5.68	126.52	120.10	17	1
1	A	131	THR	N-CA-CB	-5.68	102.71	111.46	14	2
1	A	5	PHE	O-C-N	-5.67	116.31	123.17	5	2
1	A	35	TRP	CE2-CD2-CG	5.67	114.00	107.20	20	1
1	A	39	ASN	CA-CB-CG	5.67	118.27	112.60	9	2
1	A	57	ASN	CA-C-O	-5.66	115.43	121.94	1	1
1	A	16	ILE	CA-CB-CG1	5.66	120.03	110.40	4	1
1	A	115	ASP	CA-C-N	5.66	125.37	119.82	17	2
1	A	115	ASP	C-N-CA	5.66	125.37	119.82	17	2
1	A	113	ASN	N-CA-CB	-5.66	102.02	110.17	14	2
1	A	8	ALA	CA-C-N	5.66	128.32	120.29	20	2
1	A	8	ALA	C-N-CA	5.66	128.32	120.29	20	2
1	A	67	THR	CA-C-O	-5.65	111.87	119.11	2	1
1	A	86	ILE	CA-C-N	5.65	129.37	122.42	17	2
1	A	86	ILE	C-N-CA	5.65	129.37	122.42	17	2
1	A	23	CYS	CA-C-O	-5.65	113.87	120.20	3	1
1	A	132	THR	CA-C-O	-5.65	114.50	121.06	8	1
1	A	74	SER	O-C-N	-5.65	116.14	122.75	11	1
1	A	28	ARG	NE-CZ-NH2	5.65	124.28	119.20	18	1
1	A	48	PHE	CA-CB-CG	-5.65	108.15	113.80	11	1
1	A	133	ILE	N-CA-CB	5.64	121.09	111.50	18	1
1	A	125	VAL	N-CA-C	5.64	113.81	109.19	9	1
1	A	4	GLN	O-C-N	5.63	129.30	122.20	11	2
1	A	33	TYR	CA-C-N	5.63	132.45	121.63	17	1
1	A	33	TYR	C-N-CA	5.63	132.45	121.63	17	1
1	A	85	LEU	N-CA-C	5.63	118.31	108.52	13	1
1	A	49	ALA	N-CA-C	5.63	117.86	111.11	18	2
1	A	112	ASP	N-CA-CB	-5.62	102.51	111.62	11	2
1	A	124	VAL	CA-C-O	-5.61	114.77	121.28	16	2
1	A	91	GLN	CA-C-N	5.61	129.44	121.42	5	1
1	A	91	GLN	C-N-CA	5.61	129.44	121.42	5	1
1	A	57	ASN	O-C-N	-5.60	116.07	122.68	9	2
1	A	96	CYS	CA-C-N	5.58	132.02	121.69	12	2
1	A	96	CYS	C-N-CA	5.58	132.02	121.69	12	2
1	A	70	ASN	CA-CB-CG	5.58	118.18	112.60	14	1
1	A	3	PRO	CB-CA-C	-5.58	103.93	111.85	3	2
1	A	128	HIS	N-CA-CB	-5.58	102.35	111.66	7	1
1	A	62	CYS	N-CA-CB	-5.58	103.02	110.77	16	1
1	A	51	VAL	CA-C-O	-5.57	115.26	121.17	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	81	LEU	N-CA-C	5.57	118.04	109.07	19	1
1	A	72	HIS	CE1-NE2-CD2	-5.56	103.44	109.00	4	2
1	A	19	ASN	CA-C-O	-5.56	114.70	121.15	19	1
1	A	83	CYS	O-C-N	-5.55	115.67	123.11	18	1
1	A	68	LEU	CA-C-O	5.55	125.00	118.90	18	1
1	A	113	ASN	CB-CG-ND2	5.55	124.72	116.40	17	1
1	A	10	TRP	CA-C-N	5.55	128.03	120.54	19	1
1	A	10	TRP	C-N-CA	5.55	128.03	120.54	19	1
1	A	60	ILE	CA-C-N	5.54	131.71	122.73	9	1
1	A	60	ILE	C-N-CA	5.54	131.71	122.73	9	1
1	A	7	ARG	N-CA-C	-5.54	105.25	112.23	10	1
1	A	60	ILE	CA-CB-CG1	5.54	119.81	110.40	2	1
1	A	61	ARG	CA-C-O	-5.54	114.98	121.46	2	1
1	A	64	HIS	CE1-NE2-CD2	-5.53	103.47	109.00	8	1
1	A	111	CYS	CA-C-N	5.52	131.15	122.21	9	1
1	A	111	CYS	C-N-CA	5.52	131.15	122.21	9	1
1	A	56	GLY	CA-C-N	5.51	130.54	121.39	11	1
1	A	56	GLY	C-N-CA	5.51	130.54	121.39	11	1
1	A	50	ASN	N-CA-C	5.51	117.36	111.36	4	1
1	A	99	ALA	CA-C-N	5.51	129.38	121.50	11	3
1	A	99	ALA	C-N-CA	5.51	129.38	121.50	11	3
1	A	104	ARG	NH1-CZ-NH2	-5.51	112.14	119.30	11	2
1	A	128	HIS	ND1-CG-CD2	5.51	111.61	106.10	4	1
1	A	36	ARG	CA-C-O	-5.50	115.19	121.40	18	2
1	A	22	ARG	NH1-CZ-NH2	-5.50	112.16	119.30	1	3
1	A	133	ILE	CB-CG1-CD1	5.49	125.32	113.80	13	2
1	A	42	THR	OG1-CB-CG2	-5.48	98.34	109.30	14	1
1	A	37	CYS	CA-C-N	5.47	131.56	121.94	20	3
1	A	37	CYS	C-N-CA	5.47	131.56	121.94	20	3
1	A	53	ASN	CA-C-N	5.46	128.17	120.42	18	1
1	A	53	ASN	C-N-CA	5.46	128.17	120.42	18	1
1	A	10	TRP	CB-CA-C	5.46	121.15	110.67	6	1
1	A	108	VAL	CA-C-N	5.45	131.28	123.27	11	1
1	A	108	VAL	C-N-CA	5.45	131.28	123.27	11	1
1	A	43	PHE	CA-C-O	-5.44	114.96	121.11	20	1
1	A	30	ILE	CA-CB-CG1	5.44	119.65	110.40	13	1
1	A	116	PRO	CA-N-CD	-5.43	104.39	112.00	19	1
1	A	55	CYS	N-CA-C	5.43	119.53	113.01	2	1
1	A	53	ASN	CB-CG-ND2	5.43	124.54	116.40	20	1
1	A	102	PRO	CA-C-O	-5.42	115.39	122.12	1	1
1	A	21	PRO	N-CD-CG	5.41	111.31	103.20	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	131	THR	OG1-CB-CG2	-5.41	98.48	109.30	3	1
1	A	35	TRP	CA-C-O	-5.41	113.75	119.97	19	1
1	A	12	ALA	O-C-N	5.41	127.93	122.09	20	2
1	A	82	HIS	CA-CB-CG	-5.41	108.39	113.80	6	1
1	A	40	GLN	CA-CB-CG	5.41	124.91	114.10	18	1
1	A	101	ARG	O-C-N	-5.40	116.51	121.42	17	1
1	A	26	ALA	CA-C-N	5.40	128.05	120.28	1	1
1	A	26	ALA	C-N-CA	5.40	128.05	120.28	1	1
1	A	28	ARG	O-C-N	-5.38	115.92	122.22	16	1
1	A	32	ASN	CA-C-O	5.38	125.28	119.15	19	2
1	A	124	VAL	CA-CB-CG2	5.38	119.54	110.40	17	1
1	A	126	PRO	CA-C-O	-5.37	115.04	121.48	9	1
1	A	121	ARG	O-C-N	5.37	129.37	122.39	2	1
1	A	125	VAL	CA-CB-CG1	5.37	119.53	110.40	16	1
1	A	95	ASN	CB-CA-C	5.36	116.08	109.16	4	1
1	A	45	ARG	CB-CA-C	5.36	120.05	111.91	9	1
1	A	80	LEU	O-C-N	-5.36	117.93	123.29	13	1
1	A	71	CYS	CA-C-O	-5.36	115.72	121.45	1	1
1	A	63	PRO	CB-CA-C	-5.36	103.35	111.44	6	1
1	A	2	PRO	CA-C-O	-5.35	112.80	120.56	2	1
1	A	61	ARG	CB-CA-C	5.35	120.04	109.66	3	1
1	A	34	ARG	CD-NE-CZ	5.35	131.89	124.40	11	2
1	A	2	PRO	O-C-N	5.34	127.76	121.46	7	1
1	A	33	TYR	O-C-N	-5.34	116.27	122.09	13	1
1	A	81	LEU	N-CA-CB	-5.34	101.71	110.68	3	1
1	A	104	ARG	NE-CZ-NH2	5.33	124.00	119.20	13	1
1	A	31	ASN	N-CA-C	5.33	119.65	113.20	16	2
1	A	98	TYR	CA-C-N	5.33	130.91	121.80	1	1
1	A	98	TYR	C-N-CA	5.33	130.91	121.80	1	1
1	A	44	LEU	O-C-N	5.33	129.26	123.13	13	1
1	A	107	TYR	N-CA-CB	-5.33	103.15	111.56	5	1
1	A	79	PRO	N-CD-CG	5.33	111.19	103.20	12	1
1	A	89	GLY	CA-C-O	-5.32	111.31	120.57	10	1
1	A	20	PRO	CA-C-O	5.32	124.93	120.73	3	1
1	A	67	THR	N-CA-CB	5.32	117.72	110.01	7	1
1	A	44	LEU	CA-C-N	5.32	130.08	122.21	11	1
1	A	44	LEU	C-N-CA	5.32	130.08	122.21	11	1
1	A	112	ASP	CA-C-N	5.31	128.26	120.71	10	2
1	A	112	ASP	C-N-CA	5.31	128.26	120.71	10	2
1	A	22	ARG	CA-C-O	5.31	126.99	121.15	6	1
1	A	48	PHE	N-CA-C	5.31	117.82	111.71	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	GLN	N-CA-C	5.31	117.73	110.24	5	1
1	A	107	TYR	N-CA-C	5.30	117.25	109.24	4	1
1	A	103	GLY	CA-C-O	-5.30	116.23	121.48	8	1
1	A	64	HIS	CB-CG-ND1	5.30	130.65	122.70	15	1
1	A	47	THR	N-CA-C	5.29	117.96	110.50	16	1
1	A	122	TYR	N-CA-C	5.29	120.09	108.66	16	1
1	A	50	ASN	N-CA-CB	-5.29	102.39	110.07	19	1
1	A	9	GLN	O-C-N	-5.29	116.12	122.15	10	1
1	A	81	LEU	CA-C-O	5.29	126.65	120.20	11	2
1	A	55	CYS	O-C-N	5.29	128.41	122.22	15	1
1	A	7	ARG	N-CA-CB	-5.29	102.09	110.28	17	1
1	A	17	SER	CB-CA-C	-5.28	103.73	111.23	12	1
1	A	66	ARG	N-CA-CB	5.28	117.88	110.12	3	1
1	A	114	ARG	NE-CZ-NH1	5.28	126.78	121.50	4	3
1	A	53	ASN	CB-CA-C	5.27	119.64	110.68	20	1
1	A	27	MET	N-CA-CB	5.27	119.14	110.39	18	1
1	A	22	ARG	CA-C-N	5.26	128.06	120.38	16	2
1	A	22	ARG	C-N-CA	5.26	128.06	120.38	16	2
1	A	52	VAL	N-CA-C	5.25	117.62	111.05	1	1
1	A	74	SER	CA-C-N	5.25	127.32	120.28	5	1
1	A	74	SER	C-N-CA	5.25	127.32	120.28	5	1
1	A	45	ARG	CA-C-N	5.25	130.45	122.11	11	1
1	A	45	ARG	C-N-CA	5.25	130.45	122.11	11	1
1	A	22	ARG	O-C-N	-5.24	116.61	122.75	9	1
1	A	25	ILE	N-CA-CB	-5.24	104.72	111.90	17	1
1	A	67	THR	N-CA-C	5.24	119.15	112.87	16	1
1	A	74	SER	N-CA-C	5.23	117.81	110.23	4	1
1	A	20	PRO	CA-N-CD	-5.23	104.68	112.00	5	1
1	A	96	CYS	CA-C-O	5.22	126.66	120.96	19	1
1	A	36	ARG	NE-CZ-NH1	5.22	126.72	121.50	4	1
1	A	132	THR	O-C-N	-5.22	117.20	123.31	13	1
1	A	113	ASN	O-C-N	-5.22	116.70	122.86	14	1
1	A	79	PRO	CA-C-O	5.22	126.98	121.03	7	1
1	A	77	ARG	CD-NE-CZ	5.22	131.70	124.40	16	1
1	A	63	PRO	CA-N-CD	-5.21	104.70	112.00	12	1
1	A	128	HIS	CA-C-O	-5.21	114.28	120.43	3	1
1	A	49	ALA	CA-C-N	5.21	127.26	120.28	1	1
1	A	49	ALA	C-N-CA	5.21	127.26	120.28	1	1
1	A	83	CYS	CA-C-O	5.21	126.65	120.66	2	1
1	A	30	ILE	O-C-N	-5.21	116.66	121.97	16	2
1	A	78	VAL	N-CA-CB	5.21	118.50	111.21	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	40	GLN	N-CA-C	5.20	117.15	108.99	10	1
1	A	9	GLN	N-CA-C	-5.19	105.53	111.14	17	1
1	A	6	THR	N-CA-C	-5.19	103.68	110.53	7	1
1	A	2	PRO	CB-CA-C	5.19	117.25	110.92	19	1
1	A	88	PRO	CA-C-N	5.18	131.56	121.41	15	2
1	A	88	PRO	C-N-CA	5.18	131.56	121.41	15	2
1	A	26	ALA	N-CA-CB	-5.18	102.25	110.28	10	1
1	A	26	ALA	N-CA-C	5.18	117.82	111.82	8	1
1	A	10	TRP	CD2-CE2-CZ2	5.18	127.58	122.40	20	1
1	A	121	ARG	CA-C-N	5.17	131.97	123.08	16	1
1	A	121	ARG	C-N-CA	5.17	131.97	123.08	16	1
1	A	97	ARG	CA-C-O	5.17	126.78	120.99	13	1
1	A	6	THR	N-CA-CB	5.16	118.14	110.29	11	1
1	A	83	CYS	CA-C-N	5.16	130.01	121.86	18	1
1	A	83	CYS	C-N-CA	5.16	130.01	121.86	18	1
1	A	75	ARG	CA-C-O	5.16	125.73	119.49	6	1
1	A	41	ASN	N-CA-C	5.15	116.90	109.07	1	1
1	A	28	ARG	N-CA-C	-5.15	105.79	111.71	10	2
1	A	74	SER	CA-C-O	5.14	127.17	121.56	13	1
1	A	37	CYS	N-CA-C	5.14	116.97	110.33	20	1
1	A	60	ILE	CA-C-O	-5.14	116.43	121.67	11	1
1	A	104	ARG	N-CA-C	5.14	116.69	107.80	1	1
1	A	35	TRP	CG-CD2-CE3	-5.14	128.76	133.90	12	1
1	A	42	THR	CA-C-O	-5.14	114.61	120.32	13	1
1	A	109	VAL	N-CA-C	5.14	116.10	108.65	13	1
1	A	36	ARG	O-C-N	-5.13	115.95	122.78	2	1
1	A	80	LEU	CD1-CG-CD2	-5.13	99.51	110.80	8	1
1	A	129	LEU	N-CA-CB	-5.13	102.19	110.81	16	1
1	A	43	PHE	CA-C-N	5.13	129.42	122.19	11	1
1	A	43	PHE	C-N-CA	5.13	129.42	122.19	11	1
1	A	88	PRO	CA-N-CD	-5.13	104.82	112.00	2	1
1	A	43	PHE	O-C-N	-5.13	117.11	123.36	7	1
1	A	100	ASP	N-CA-CB	5.12	117.88	109.95	11	1
1	A	12	ALA	CA-C-N	5.12	127.47	120.46	11	1
1	A	12	ALA	C-N-CA	5.12	127.47	120.46	11	1
1	A	69	ASN	CB-CA-C	5.11	119.69	111.36	6	1
1	A	22	ARG	N-CA-CB	5.11	117.53	110.17	1	1
1	A	24	THR	CA-CB-CG2	5.11	119.18	110.50	6	1
1	A	69	ASN	N-CA-C	5.10	118.48	111.54	13	1
1	A	117	ARG	CA-CB-CG	-5.10	103.90	114.10	8	1
1	A	119	SER	N-CA-C	5.10	121.08	109.81	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	PRO	CA-C-O	-5.10	111.32	120.60	15	1
1	A	101	ARG	CA-CB-CG	5.10	124.29	114.10	2	1
1	A	4	GLN	CA-CB-CG	5.10	124.29	114.10	3	1
1	A	89	GLY	N-CA-C	5.09	118.84	112.73	2	1
1	A	120	PRO	N-CA-CB	5.09	109.00	103.30	1	1
1	A	79	PRO	N-CA-CB	5.08	107.77	103.35	4	1
1	A	72	HIS	N-CA-CB	-5.08	103.54	111.56	20	1
1	A	93	ILE	CA-C-O	-5.07	114.44	120.78	14	1
1	A	35	TRP	O-C-N	-5.06	115.81	122.39	7	1
1	A	20	PRO	N-CD-CG	5.05	110.77	103.20	12	1
1	A	21	PRO	CA-C-N	5.04	128.01	120.90	12	2
1	A	21	PRO	C-N-CA	5.04	128.01	120.90	12	2
1	A	96	CYS	N-CA-C	5.04	117.47	109.96	2	1
1	A	68	LEU	O-C-N	-5.04	116.59	121.93	5	1
1	A	70	ASN	N-CA-CB	-5.04	102.01	110.32	12	1
1	A	44	LEU	N-CA-C	5.03	116.98	109.59	1	1
1	A	118	ASP	CA-CB-CG	5.03	117.63	112.60	20	1
1	A	44	LEU	CA-C-O	-5.03	114.86	120.54	11	1
1	A	39	ASN	CB-CG-ND2	5.03	123.94	116.40	7	1
1	A	125	VAL	CG1-CB-CG2	-5.02	99.76	110.80	16	1
1	A	20	PRO	N-CA-C	5.01	116.82	110.70	5	1
1	A	131	THR	N-CA-C	5.01	115.76	108.14	17	1
1	A	127	VAL	CB-CA-C	-5.01	103.08	111.29	4	1
1	A	122	TYR	N-CA-CB	5.00	118.17	110.12	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	TYR	Sidechain	9
1	A	5	PHE	Sidechain,Peptide	8
1	A	22	ARG	Sidechain	5
1	A	11	PHE	Sidechain	4
1	A	34	ARG	Sidechain,Mainchain	4
1	A	66	ARG	Sidechain	4
1	A	75	ARG	Sidechain	4
1	A	106	PHE	Sidechain	4
1	A	114	ARG	Sidechain,Peptide	4
1	A	33	TYR	Sidechain	4
1	A	45	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	ARG	Sidechain	4
1	A	117	ARG	Sidechain	4
1	A	104	ARG	Sidechain	4
1	A	122	TYR	Sidechain,Mainchain	4
1	A	28	ARG	Sidechain	3
1	A	105	ARG	Sidechain	3
1	A	43	PHE	Mainchain,Sidechain	3
1	A	36	ARG	Sidechain,Mainchain	3
1	A	98	TYR	Sidechain	2
1	A	18	LEU	Peptide,Mainchain	2
1	A	64	HIS	Peptide	2
1	A	14	GLN	Mainchain,Peptide	2
1	A	7	ARG	Sidechain	2
1	A	97	ARG	Sidechain	2
1	A	83	CYS	Peptide	2
1	A	29	ALA	Mainchain	1
1	A	82	HIS	Sidechain	1
1	A	99	ALA	Peptide	1
1	A	76	PHE	Sidechain	1
1	A	91	GLN	Mainchain	1
1	A	73	ARG	Sidechain	1
1	A	70	ASN	Sidechain	1
1	A	13	ILE	Mainchain	1
1	A	77	ARG	Sidechain	1
1	A	101	ARG	Sidechain	1
1	A	2	PRO	Peptide	1
1	A	78	VAL	Peptide	1
1	A	87	ASN	Sidechain	1
1	A	6	THR	Peptide	1
1	A	129	LEU	Peptide	1
1	A	61	ARG	Sidechain	1
1	A	21	PRO	Peptide	1
1	A	48	PHE	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1083	1060	1055	1±1
2	B	58	32	12	0±0
All	All	22820	21840	21347	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LEU:HD12	1:A:80:LEU:C	0.56	2.25	19	1
1:A:107:TYR:HB3	1:A:132:THR:HG22	0.53	1.79	13	1
1:A:128:HIS:CD2	1:A:129:LEU:H	0.47	2.28	17	1
1:A:60:ILE:HG13	1:A:71:CYS:SG	0.46	2.49	20	1
1:A:100:ASP:C	1:A:101:ARG:HD2	0.45	2.37	6	1
1:A:23:CYS:SG	1:A:100:ASP:HA	0.44	2.52	1	2
1:A:38:LYS:HE2	2:B:3:SGN:N2	0.43	2.29	1	1
1:A:108:VAL:O	1:A:129:LEU:HD12	0.42	2.14	11	1
1:A:26:ALA:HB1	1:A:43:PHE:CZ	0.42	2.49	4	1
1:A:38:LYS:HE2	2:B:3:SGN:H3	0.42	1.91	3	1
1:A:41:ASN:ND2	1:A:43:PHE:CE1	0.41	2.89	8	1
1:A:27:MET:HG3	1:A:98:TYR:CD1	0.41	2.51	3	1
1:A:72:HIS:O	1:A:108:VAL:HG13	0.40	2.16	20	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/133 (98%)	113±4 (87±3%)	16±3 (12±3%)	2±1 (1±1%)	13	61
All	All	2620/2660 (98%)	2267 (87%)	322 (12%)	31 (1%)	13	61

All 21 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	86	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	24	THR	3
1	A	102	PRO	3
1	A	88	PRO	2
1	A	89	GLY	2
1	A	3	PRO	2
1	A	85	LEU	2
1	A	121	ARG	1
1	A	127	VAL	1
1	A	20	PRO	1
1	A	120	PRO	1
1	A	55	CYS	1
1	A	95	ASN	1
1	A	96	CYS	1
1	A	4	GLN	1
1	A	15	HIS	1
1	A	79	PRO	1
1	A	58	GLN	1
1	A	12	ALA	1
1	A	68	LEU	1
1	A	66	ARG	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/122 (99%)	117±1 (97±1%)	4±1 (3±1%)	36	85
All	All	2420/2440 (99%)	2346 (97%)	74 (3%)	36	85

All 27 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	133	ILE	20
1	A	30	ILE	8
1	A	51	VAL	6
1	A	86	ILE	4
1	A	80	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	122	TYR	3
1	A	88	PRO	3
1	A	19	ASN	3
1	A	25	ILE	2
1	A	35	TRP	2
1	A	124	VAL	2
1	A	3	PRO	2
1	A	67	THR	2
1	A	100	ASP	1
1	A	46	THR	1
1	A	43	PHE	1
1	A	129	LEU	1
1	A	76	PHE	1
1	A	21	PRO	1
1	A	109	VAL	1
1	A	52	VAL	1
1	A	130	ASP	1
1	A	10	TRP	1
1	A	121	ARG	1
1	A	6	THR	1
1	A	60	ILE	1
1	A	125	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	LVZ	B	1	2	23,23,23	1.89±0.30	6±1 (25±5%)
2	IDS	B	2	2	16,16,17	1.89±0.34	4±1 (25±9%)
2	SGN	B	3	2	19,19,20	1.90±0.45	5±2 (25±8%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	LVZ	B	1	2	28,35,35	1.88±0.28	6±2 (22±7%)
2	IDS	B	2	2	16,24,26	1.69±0.37	3±1 (20±9%)
2	SGN	B	3	2	23,29,31	2.05±0.33	7±2 (28±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LVZ	B	1	2	-	0±0,15,35,35	0±0,1,1,1
2	IDS	B	2	2	-	0±0,9,26,29	0±0,1,1,1
2	SGN	B	3	2	-	0±0,11,28,31	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	3	SGN	S1-N2	8.36	1.70	1.59	1	17
2	B	1	LVZ	S19-N9	8.16	1.69	1.59	3	12
2	B	3	SGN	O1S-S1	7.12	1.50	1.42	4	7
2	B	2	IDS	O5-C1	6.76	1.55	1.43	8	12
2	B	2	IDS	C1-C2	6.43	1.62	1.51	10	9
2	B	1	LVZ	O5-C5	6.08	1.59	1.44	20	9
2	B	1	LVZ	O3S-S19	5.74	1.48	1.42	6	14
2	B	2	IDS	O5-C5	5.45	1.54	1.43	15	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	3	SGN	O2S-S1	5.21	1.48	1.42	17	13
2	B	1	LVZ	O2S-S19	4.72	1.47	1.42	9	10
2	B	1	LVZ	O5-C1	4.67	1.53	1.41	13	9
2	B	3	SGN	O5-C5	4.62	1.52	1.43	6	9
2	B	1	LVZ	C2-N9	4.58	1.53	1.47	12	11
2	B	2	IDS	C4-C5	4.55	1.60	1.53	18	11
2	B	2	IDS	C5-C6	4.55	1.62	1.53	20	5
2	B	1	LVZ	O1-C1	4.46	1.54	1.41	15	9
2	B	1	LVZ	O4-C4	4.44	1.53	1.43	20	11
2	B	2	IDS	O4-C4	4.39	1.53	1.43	16	7
2	B	1	LVZ	C1-C2	4.15	1.59	1.53	6	7
2	B	3	SGN	C2-N2	4.11	1.54	1.47	1	8
2	B	2	IDS	C4-C3	4.06	1.62	1.52	1	1
2	B	2	IDS	O2-C2	3.99	1.53	1.47	10	2
2	B	3	SGN	C1-C2	3.85	1.57	1.52	8	6
2	B	1	LVZ	C3-C2	3.68	1.46	1.53	15	7
2	B	3	SGN	O5-C1	3.54	1.49	1.43	4	14
2	B	2	IDS	O6B-C6	3.49	1.19	1.30	16	8
2	B	2	IDS	C3-C2	3.43	1.60	1.53	20	5
2	B	2	IDS	O2-S	3.42	1.47	1.57	2	2
2	B	1	LVZ	C6-C5	3.13	1.61	1.51	8	2
2	B	3	SGN	C4-C5	3.08	1.59	1.53	16	7
2	B	1	LVZ	C4-C5	3.08	1.59	1.53	15	5
2	B	3	SGN	O4-C4	3.07	1.50	1.43	9	5
2	B	3	SGN	O6-S2	2.91	1.64	1.56	10	2
2	B	2	IDS	O6A-C6	2.80	1.30	1.22	5	1
2	B	2	IDS	O3-C3	2.68	1.36	1.43	15	1
2	B	3	SGN	C6-C5	2.62	1.59	1.51	12	5
2	B	3	SGN	O3-C3	2.47	1.49	1.43	1	2
2	B	1	LVZ	O3-C3	2.43	1.49	1.43	8	1
2	B	1	LVZ	O6-S29	2.40	1.50	1.56	4	4
2	B	1	LVZ	C4-C3	2.38	1.58	1.52	5	3
2	B	1	LVZ	C3A-C1A	2.16	1.61	1.49	1	1
2	B	1	LVZ	C2A-C1A	2.13	1.60	1.49	4	1
2	B	3	SGN	C3-C2	2.01	1.56	1.52	14	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	3	SGN	C1-O5-C5	8.98	124.22	112.19	10	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	1	LVZ	O3S-S19-N9	7.85	95.75	108.88	4	14
2	B	2	IDS	O2-C2-C3	7.49	117.42	106.95	10	9
2	B	2	IDS	C4-C3-C2	6.52	122.06	110.23	10	12
2	B	1	LVZ	O2S-S19-O3S	6.45	106.01	120.36	6	20
2	B	3	SGN	C3-C4-C5	6.01	121.13	110.23	20	8
2	B	3	SGN	C3-C2-N2	5.89	118.06	110.32	15	10
2	B	1	LVZ	O6-C6-C5	5.71	117.75	107.57	17	8
2	B	3	SGN	O5-C1-C2	5.70	102.47	111.29	10	1
2	B	3	SGN	O1S-S1-O2S	5.51	108.10	120.36	15	18
2	B	1	LVZ	C4-C3-C2	5.47	118.37	110.40	15	8
2	B	1	LVZ	O1-C1-C2	5.38	116.81	108.07	18	7
2	B	3	SGN	C1-C2-N2	5.13	118.34	110.22	6	9
2	B	1	LVZ	O2S-S19-N9	4.96	117.18	108.88	8	7
2	B	1	LVZ	C3-C4-C5	4.92	101.31	110.23	14	7
2	B	1	LVZ	C1-C2-N9	4.69	118.70	110.91	19	10
2	B	3	SGN	O6-C6-C5	4.67	115.89	107.57	1	7
2	B	3	SGN	O1S-S1-N2	4.64	101.12	108.88	17	10
2	B	2	IDS	C3-C4-C5	4.57	117.17	109.30	15	10
2	B	1	LVZ	O5-C5-C6	4.46	115.55	106.69	19	8
2	B	1	LVZ	C6-C5-C4	4.38	121.26	112.07	17	4
2	B	2	IDS	O5-C5-C6	4.13	121.34	106.59	3	11
2	B	3	SGN	O3-C3-C2	3.91	101.28	109.40	6	8
2	B	1	LVZ	O3-C3-C2	3.82	101.97	109.58	12	4
2	B	3	SGN	C4-C3-C2	3.75	105.52	111.02	3	5
2	B	1	LVZ	O5-C1-C2	3.65	103.70	110.59	18	3
2	B	3	SGN	O2S-S1-N2	3.52	114.77	108.88	8	5
2	B	3	SGN	O4-C4-C3	3.49	102.15	110.38	3	9
2	B	3	SGN	O4-C4-C5	3.38	117.66	109.32	11	3
2	B	2	IDS	O3S-S-O1S	3.38	120.38	108.56	13	1
2	B	3	SGN	O5-C5-C4	3.33	102.72	110.83	12	2
2	B	1	LVZ	O5-C5-C4	3.33	103.70	109.70	7	7
2	B	2	IDS	O3-C3-C2	3.31	101.17	109.32	19	7
2	B	1	LVZ	O4-C4-C3	3.26	102.70	110.38	11	8
2	B	2	IDS	O4-C4-C5	3.19	117.03	109.76	20	1
2	B	3	SGN	O3-C3-C4	3.08	103.11	110.38	18	4
2	B	2	IDS	O3-C3-C4	3.07	103.14	110.38	8	3
2	B	1	LVZ	O3-C3-C4	3.05	103.18	110.38	15	4
2	B	1	LVZ	C1-O5-C5	2.97	119.51	113.72	8	1
2	B	3	SGN	O6S-S2-O6	2.96	113.17	106.37	19	3
2	B	3	SGN	O5-C5-C6	2.95	101.21	107.59	6	6
2	B	2	IDS	O6B-C6-C5	2.94	124.24	113.64	13	3

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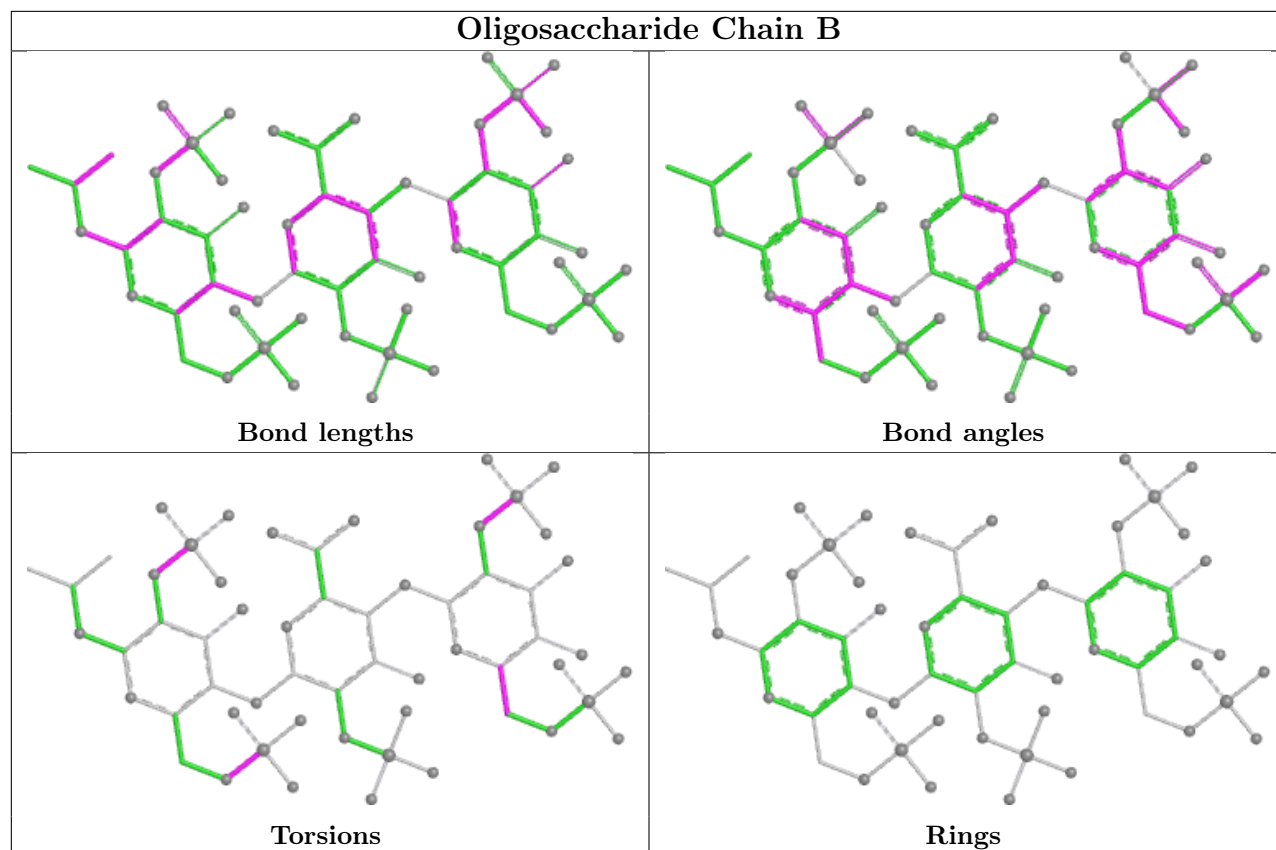
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	3	SGN	O6S-S2-O5S	2.92	118.77	108.56	11	3
2	B	2	IDS	O6B-C6-O6A	2.86	117.60	124.08	9	4
2	B	1	LVZ	O6-S29-O4S	2.73	98.57	106.92	9	1
2	B	2	IDS	O4-C4-C3	2.40	116.04	110.38	1	1
2	B	2	IDS	O3S-S-O2	2.37	111.81	106.37	8	1
2	B	2	IDS	O5-C1-C2	2.30	104.85	109.51	11	1
2	B	1	LVZ	C1-C2-C3	2.23	116.34	110.19	19	2
2	B	3	SGN	C6-C5-C4	2.19	107.47	112.07	11	3
2	B	1	LVZ	O4-C4-C5	2.16	104.00	109.32	11	2
2	B	1	LVZ	O5S-S29-O6S	2.13	116.02	108.56	16	1
2	B	2	IDS	O3S-S-O2S	2.10	115.91	108.56	6	1
2	B	2	IDS	O6A-C6-C5	2.10	113.24	120.81	11	1
2	B	3	SGN	O6S-S2-O4S	2.09	115.87	108.56	10	1
2	B	1	LVZ	O5S-S29-O4S	2.09	115.86	108.56	5	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1481
Number of shifts mapped to atoms	1481
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	129	-0.01 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	129	-0.09 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	120	1.12 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1470 atoms were assigned a chemical shift out of a possible 1898. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	503/639 (79%)	255/255 (100%)	128/264 (48%)	120/120 (100%)
Sidechain	888/1099 (81%)	599/707 (85%)	263/316 (83%)	26/76 (34%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	79/160 (49%)	62/78 (79%)	15/70 (21%)	2/12 (17%)
Overall	1470/1898 (77%)	916/1040 (88%)	406/650 (62%)	148/208 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1480 atoms were assigned a chemical shift out of a possible 1921. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	505/644 (78%)	256/257 (100%)	129/266 (48%)	120/121 (99%)
Sidechain	896/1117 (80%)	604/718 (84%)	266/320 (83%)	26/79 (33%)
Aromatic	79/160 (49%)	62/78 (79%)	15/70 (21%)	2/12 (17%)
Overall	1480/1921 (77%)	922/1053 (88%)	410/656 (62%)	148/212 (70%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	117	ARG	H	0.30	5.25 – 11.22	-13.3
1	A	12	ALA	CB	38.40	10.19 – 27.75	11.1
1	A	14	GLN	HG3	0.58	0.91 – 3.68	-6.2
1	A	126	PRO	HB3	0.07	0.25 – 3.76	-5.5
1	A	14	GLN	HB2	0.68	0.80 – 3.29	-5.5
1	A	74	SER	HB3	2.44	2.49 – 5.20	-5.2
1	A	27	MET	HB3	0.28	0.33 – 3.66	-5.2
1	A	77	ARG	HG3	0.15	0.15 – 2.94	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

